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Solubilization of 5- Amino Salicylic Acid in Different Micellar Media: A Fluorescence Approach

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Abstract

Objective: To develop solubilization of 5- amino salicylic acid in different micellar media for Pharmaceuticals, biological sciences, detergency, beauty products, manufacturing of textiles, engineering. **Methods:** A fluorescence approach with anionic, cationic, and nonionic micellar media were used to study the solubilization of 5-amino salicylic acid (5-ASA) at varying concentrations. Absorption spectrum measurements have also verified the solubilization phenomena. In micellar mediums with varying compound concentrations, spectral characteristics such as quantum yield, Stokes' shift, and molar extinction coefficient were computed. **Findings:** Changes in the solubilization pattern in the presence of various surfactant classes have been demonstrated by changes in the curve area and quantum yield. **Novelty:** Catalytic solvents have had the greatest impact on the solubilization of 5-amino salicylic acid in its aqueous solution. This study involved in solubilization of 5- amino salicylic acid in different micellar media surfactant-based separations, chemical analysis, emulsion, polymerisation, micellar catalysis, and environmental processes are just a new of the fields that have used solubilization.

Keywords: 5- Amino Salicylic acid (5-ASA); Solubilization; Micellar media; Spectral parameters; Quantum yield

1 Introduction

In order to develop a thermodynamically stable isotropic solution with decreased thermodynamic activity of the solubilized material, a substance (solid, liquid, or gas) must spontaneously dissolve by reversible interaction with the micelles of a surfactant in a solvent. In other words, adding surfactants to solutions increases the solubility of mostly hydrophobic molecules in aqueous solution. By giving the sparingly soluble molecules a more favorable environment, the additional surfactant molecule self-assembles to create micelles or vesicles, increasing the solubilization of the molecules. Many industries, including food, cleaning supplies, paints, cosmetics, oil recovery, wastewater treatment, different separation processes, and the pharmaceutical sector, have made extensive use of surfactants. Moradi et al., studied on solubility

of 5-aminosalicylic acid in {N-methyl-2-pyrrolidone + ethanol} mixtures at T = (293.2 to 313.2) K[1]. 5-Aminosalicylic acid (5-ASA), also known as Mesalamine, is an anti-inflammatory drug. Several new 5-aminosalicylic acid (5-ASA) derivatives have been introduced and enhanced topical delivery of salicylic acid via hydrotropic solubilization technique: Formulation and evaluation of solution and gel systems for topical application[2]. This approach allows for solubilization investigations at low concentrations. The chemical nature of fluorescence and stimulating radiation causes high sensitivity of Novel 5-aminosalicylic derivatives as anti-inflammatories and myeloperoxidase inhibitors and eco-friendly synchronous spectrofluorimetric method for simultaneous determination of remdesivir and acetyl salicylic acid in spiked human plasma[3]. Fluorescent probes as a tool in diagnostic and drug delivery systems[4] and is the most effective technique for determining the critical micellar concentration and tracking the relationship between surfactants and molecules of organic matter because of its high sensitivity. Ojha et al., (2021) reported on pharmaceutical aspects of micellar solubilization of salicylic acids using different surfactants[5], as micelle production, also known as micellization, is a fascinating chemical phenomenon that has significant medical and economic applications. Micelles are especially important in pharmacy because they can make sparingly soluble compounds more soluble in water as construction of A ratio fluorescence assay of 5- Amino salicylic acid based on its aggregation induced emission with blue emitting N/P-codoped carbon dots[6]. Lal M reported on innovative study for enhanced performance of surfactants as they have a tendency to associate in solution, forming particles of colloidal dimension called micelles, which get adsorbed at interfaces[7]. Numerous fields, including the field of "Novel 5-aminosalicylic derivatives as anti-inflammatories and myeloperoxidase inhibitors evaluated in silico, in vitro and ex vivo[8]. The structure, function, and quantities of surfactant, and ions have been greatly aided by recent research work[9]. The current research work examines how different nonionic, anionic, and cationic surfactants affect and reported innovative study in renewable energy source through mixed surfactant system for eco-friendly environment[10]. Hydrophobic and weakly polar organic solutes have also been examined for their effect on micelles Interaction of salicylic acid analogues with Pluronic® micelles: Investigations on micellar growth and morphological transition[11]. The solubility data of 5-amino salicylic acid in methanol, ethanol, carbon tetrachloride, and tetrahydrofuran (THF) at various temperatures were measured by gravimetrical method from (293.15 to 313.15) K under atmospheric pressure, and the solubility data were correlated as a function of temperature[12].

Solubilization of 5- amino salicylic acid in different micellar media in surfactant solutions are observed in the presence of solubility of isophthalic acid and m-toluic acid in eight monobasic alcohols: experimental measurements and thermodynamic modeling[13]. While highly polar substances like equilibrium solubility investigation and thermodynamic aspects of paracetamol, salicylic acid and 5-aminosalicylic acid in polyethylene glycol dimethyl ether 250 + water mixtures[14], and measurement and correlation of the solubility of 4-aminoantipyrine in nine mono and water + ethanol mixed solvents at temperatures from (299.05 to 338.35) K[15] favour solubilization of 5- amino salicylic acid in different micellar media.

The current work examines how different nonionic, anionic, and cationic surfactants affect 5-ASA's fluorescence and absorption spectra. Calculations of the molar extinction coefficient, the quantum yield, the empirical fluorescence coefficient, and Stokes' shift at different 5-ASA concentrations have been used to interpret the data.

2 Methodology

5-Aminosalicylic acid (5-ASA) is the product of Spectro Chemicals. Surfactants such as the following were used: (A) Nonionic surfactants (i) Polyoxyethylene Tert-octyl Phenol or TX-100 (ii) Polyoxyethylene Sorbitain Monolaurate or Tween-20 (iii) Polyoxyethylene Sorbitain Monooleate, or Tween-80 (B) Anionic surfactants (i) Dodecylbenzene Sodium Sulphonate or DBSS (ii) Dioctyl Sodium Sulphosuccinate or DSSS (iii) Sodium Lauryl Sulphate or SLS (C) Cationic surfactants (i) Cetylpyridinium Chloride or CPC (ii) Cetyltrimethyl Ammonium bromide or CTAB (iii) Myristyltrimethyl Ammonium Bromide, or MTAB. Every surfactant was a product of Sigma (USA) or BDH (UK). Every experiment was conducted between 23^0 and 25^0 C or at room temperature. 5-amino salicylic acid's stock solution was made using double-distilled water. The concentration was kept at 8×10^{-5} M for the fluorescence study and 1×10^{-4} M for the absorption study. The 5-amino salicylic acid concentration was kept constant throughout the procedure. A Systronics UV-VIS Spectrophotometer was used to record the absorption spectra, and a synchronized Perkin-Elmer model 056 strip chart recorder was used to record the fluorescence spectrum. Using surface tension measurement and the drop weight approach, the critical micelle concentration (CMC) value of surfactants was calculated to assess their purity. Using anthracene solution as a reference, the total fluorescence quantum efficiency values of 5-amino salicylic acid were calculated. The fluorescence spectra for the reference and sample were recorded using the whole emission range under the same conditions.

3 Result and discussion

Maximum excitation and emission wavelengths were recorded at 330 and 490 nm, respectively, in an aqueous solution of 5-amino salicylic acid. The fluorescence experiments were conducted with cationic, anionic, and nonionic surfactants. The addition of the nonionic surfactants TX-100 and Tween-80 caused a dramatic drop in fluorescence intensity, while Tween-20 caused a gradual increase. The intensity of fluorescence gradually increased upon the addition of any anionic surfactants. The emission intensity dropped when the cationic surfactants CTAB and MTAB were first added. At greater concentrations of these surfactants, the emission intensity increased with a blue shift of 5 nm in peak position (Figure 1). On the other hand, the emission intensity displayed a decreasing order in CPC micellar medium. The fluorescence intensity peaks and minima for 5-ASA, in presence or absence of all the surfactants listed above, are displayed in Table 1. There was a peak in the absorption spectra at 300 nm. The absorbance intensified when all three nonionic surfactants were added to the 5-ASA solution. The blue shift in λ_{max} produced by TX-100 and Tween-80 was 25 nm. The absorbance increased steadily with each of the three anionic surfactants. The red shifts for DBSS and SLS were 30 nm and 25 nm, respectively. The absorbance was also raised by each of the three cationic surfactants. As the concentration of cationic, anionic, and nonionic surfactants increased, the molar extinction coefficient ($\log \varepsilon$) values also increased. Quantum yield (ϕ_f) values for nonionic surfactants TX-100 and Tween-80 added 5-ASA solution declined as the surfactant concentration increased, but with Tween-20 $\phi_f$values grew steadily. Quantum yield (ϕ_f) values raised steadily when all of the anionic surfactants were added. With cationic surfactant CPC, quantum yield (ϕ_f) values decreased, while with CTAB and MTAB $\phi_f$values first declined and then raised. Both the fluorescence intensity and the quantum yield values were parallel to the empirical fluorescence coefficient (k_f) values. When the 5-ASA solution was diluted, the Stokes' shift values stayed constant. The spectrum characteristics (quantum yield, empirical fluorescence coefficient, and molar extinction coefficient values) for the solution containing MTAB are displayed in Table 2. The computed Stokes' shift data for 5-ASA is displayed in Table 3. The results showed that fluorescence and absorption behaviour of 5-ASA were more enhanced by cationic surfactants. The highest augmentation was demonstrated by MTAB, as confirmed by absorbance, logϵ, and $\phi_f$values. Because surfactants contain polar head groups and nonpolar long chain hydrocarbons, they are important in many chemical reactions that form micelles in aqueous media. The findings indicate that compared to the system without surfactant, the system with surfactant added has a larger enhancement in emission intensity. In the area of the specific surfactant's critical micelle concentration (CMC), this solubilization process is anticipated to be most noticeable. It was found during the studies that a certain concentration range of each surfactant, which was within the cmc range of the corresponding surfactant, caused a sudden increase in the fluorescence intensity. The premicellar aggregation in the surfactant micelle may be the cause of the alterations seen below cmc in the case of an ionic surfactant. A dynamic equilibrium is usually attained when organic molecules dissolve in micellar settings, allowing for solute exchange between the micelle and the bulk phase. The micelles that are part of the surfactants are adsorbed at the interfaces and prevent the hydrophobic groups from getting into contact with water, when they are added to the aqueous solution of compound. This encourages micellization and reduces the free energy of the system. However, as the hydrophobic groups are moved from solution to the micelle in the solvent, there might be some loss of freedom associated with the micelle and, in the case of ionic surfactants, from electrostatic repulsion from other similarly charged surfactant molecules that exist in the micelle. These forces increase the free energy of the system, which opposes micellization. The balance between the elements that support and hinder micellization determines whether micellization happens in a given situation and, if it does, at what concentration of a monomeric surfactant. TX-100 and Tween-80 reduced the intensity of fluorescence in the case of 5-ASA because they formed intramolecular hydrogen bonds. As a result, the solubilizate and the surfactant micelles are unable to form an effective hydrogen bond. Furthermore, the quenching demonstrates that the molecule prefers the hydrophobic core over the hydrophilic poly (ethylene oxide) PEO shell, particularly for TX-100. It is clear that compound's fluorescence is greatly reduced in the core, as in nonaqueous solvents. This suggests that the molecule is not hydrated around the aromatic rings and Radiationless deactivation of 6-aminocoumarin from the S1-ICT state in nonspecifically interacting solvents[16]. The drop-in intersystem crossing rate may be the cause of the increase in fluorescence intensity and ϕ_f values in ionic micellar media, which show that the rates of non-radiative processes are lower in micellar systems than in water.

4 Conclusion

After interpreting and comparing the results obtained for 5-ASA, it is found that the theoretically calculated spectral parameter like molar extinction coefficient, Stokes' shift, quantum yield values and empirical fluorescence coefficient are in good agreement with experimental results. This demonstrates that the assumption was correct. Therefore, the current basic research can be used to gain a better knowledge of how phospholipids, which function as micelles in physiological fluids, assimilate a number of vital drugs in the human body.

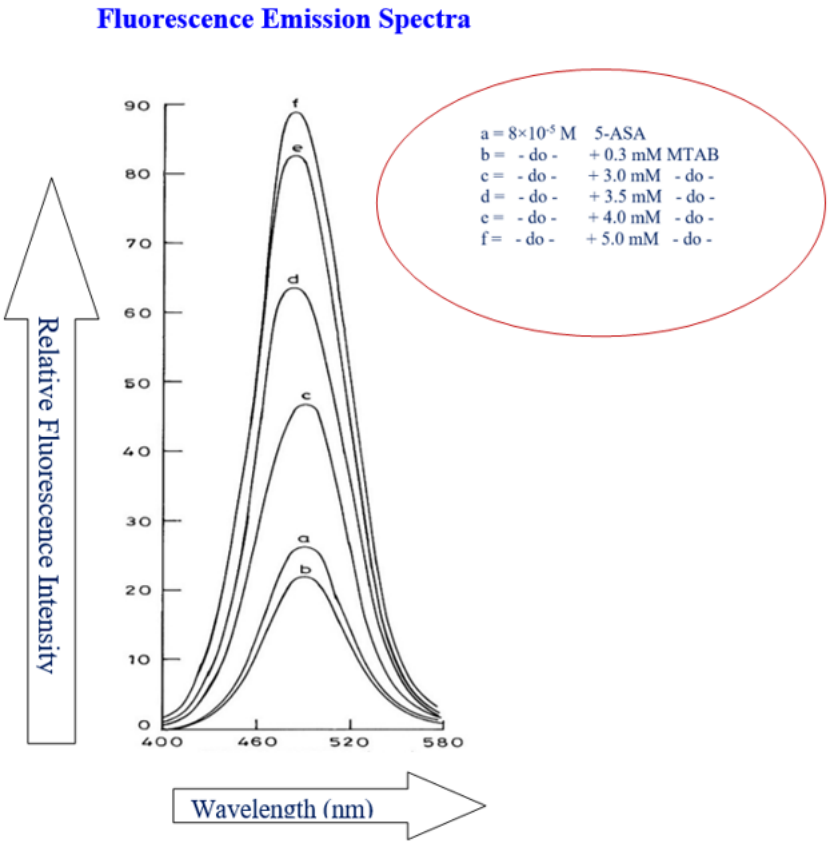

Fig 1. Fluorescence emission spectra of 5-ASA in MTAB micellar media

Table 1. Fluorescence intensity of 5-ASA in absence and presence of surfactants

S. No.	Name of surfactant	Relative fluorescence intensity in absence of surfactant	Concentration of surfactant used (mM)	Relative fluorescence intensity at max conc of surfactant	λem (nm)
1.	TX-100	26	5.0	2	490
2.	Tween-20	26	7.0	35	490
3.	Tween-80	26	5.0	6	490
4.	DBSS	26	7.0	34	490
5.	DSSS	26	7.0	38	490
6.	SLS	26	7.0	47	490
7.	CPC	26	5.0	0	490
8.	CTAB	26	5.0	91	485
9.	MTAB	26	5.0	89	485

Table 2. Absorption maxima (λ_{max}), fluorescence maxima (λ_{em}), molar extinction coefficient (log ϵ) and quantum yield (ϕ_f) of 5-ASA at different concentration of MTAB (mM)

S. No.	Concentration of MTAB used (mM)	λ_{max} (nm)	log ϵ (dm^3 mol^{-1} cm^{-1})	λ_{em} (nm)	ϕ_f
1.	0.00	300	3.6471	490	0.3468
2.	0.3	300	3.6592	490	0.2951
3.	3.0	300	3.6592	490	0.5579
4.	5.0	300	3.7252	485	1.0863

Table 3. Stokes' shift data of 5-Aminosalicylic acid at room temperature

S. No.	Conc. of compound	λ_{ex} (nm)	F.I.	λ_{em} (nm)	F.I.	P.M. Gain	Sensitivity Range	Stokes' Shift (cm^{-1})
1.	$1x10^{-3}$ M	330	99	490	47	2	1	9894
2.	$8x10^{-4}$ M	330	90	490	41	2	1	9894
3.	$6x10^{-4}$ M	330	89	490	40	2	1	9894
4.	$4x10^{-4}$ M	330	84	490	38	2	1	9894
5.	$2x10^{-4}$ M	330	74	490	34	2	1	9894
6.	$8x10^{-5}$ M	330	55	490	26	2	1	9894
7.	$6x10^{-5}$ M	330	45	490	21	2	1	9894
8.	$4x10^{-5}$ M	330	40	490	18	2	1	9894
9.	$2x10^{-5}$ M	330	24	490	11	2	1	9894

5 Data accessibility:

Every piece of information has been included in the manuscript and the addendum.

6 Declaration on the use of generative and AI-assisted AI in the while-writing process:

The authors utilised GPT 4 to enhance the document's language and readability throughout the preparation stage. Following their use of this tool/service, the writers reviewed the publication's content and made any necessary revisions, taking entirely accountable for it.

7 Author contributions statement:

The author has contributed to every aspect of this research project, including its idea, planning, data collection, analysis, interpretation, and modification. Each author has planned the study, examined the article, interpreted data, reviewed the experiments, and proofread the work for grammar and spelling errors. Additionally, the same author has participated as a corresponding author and study activity. The author has approved the version that was submitted.

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