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Quantum efficiency of aspirin spectra

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***Abstract*---**Aspirin, one of the oldest and most widely used anti-inflammatory drugs, has lately been found to lessen the incidence of cancer. The main pharmacological effects of aspirin are thought to be generated by its covalent alteration of cyclooxygenase-2 (COX-2) via acetylation of Ser530. However, the exact biochemical mechanism and specificity of how it works have yet to be figured out. In modern times, there has been a lot of research done on the qualities of spectra for pharmaceuticals (such as fluorescence), and the goal of this research is to display more physicochemical features of molecules. Anthracene is colorless, but when exposed to ultraviolet (UV) light, it fluoresces blue (with a maximum emission range of 400–450 nm). The ratio of the number of photons that are emitted to the number of photons that are absorbed can be used as a measurement of the quantum yield, which is a measurement of the efficiency of photon emission. The quantum yield ratio is the name given to this particular ratio. In the present work, we studied absorption spectra by spectrophotometer and fluorescence by spectrofluorometer photometer from UV to visible range for aspirin. We found that aspirin fluoresces (max = 370–470 nm) under UV light. So, aspirin became a sensor.

***Keywords*---**aspirin, anthracene, quantum yield, fluorescence, emission.

Introduction

Aspirin, also known as acetylsalicylic acid (ASA), is one of the most extensively used medications in the world. Despite the fact that numerous pharmaceutical studies indicate that aspirin can be used as an antithrombotic agent, it may also aid in the treatment of coronary heart and Alzheimer's illnesses and may have cancer-preventive characteristics [1]. Therefore, additional research is necessary to avoid acetylsalicylic acid's negative effects on the body [2]. As with the majority of nonsteroidal anti-inflammatory medicines (NSAIDs), aspirin's primary pharmacological molecular target is cyclooxygenase-2 (COX-2).

However, the molecular mechanism of aspirin's therapeutic activity is unique: aspirin covalently changes the COX-2 enzyme by acetylating Ser530 near its active site, preventing proper binding of the native substrate and resulting in irreversible inhibition. Aspirin can really covalently block both major isoforms of COX, however it is 10-100 times more effective against COX-1 than COX-2[3]. Since its discovery over half a century ago, the physical phenomenon of fluorescence resonance energy transfer (FRET) has found increasing application in biological research and drug development [4]. When two molecules are separated by a distance, energy is transferred between them. Molecular interactions have been studied using this technique because of its sensitivity toward distance. FRET is the transfer of energy from a donor molecule to an acceptor molecule without the need of electromagnetic radiation. As the donor molecule absorbs and transfers energy, the acceptor molecule is the chromophore to which that energy is transmitted [5]. No thermal energy is converted and no molecules collide in this resonance interaction that occurs over distances higher than the interatomic distance [6]. The donor's fluorescence intensity and excited state lifespan are reduced, while the acceptor's emission intensity is increased as a result of the transfer of energy [7]. Anthracene is a type of tricyclic aromatic hydrocarbon that may be found in coal tar. It is a starting material that is utilized in the production of dyestuffs as well as scintillation counters. Anthracene crystallizes into monoclinic plates that are colorless but emit a blue glow when it is in its purest form [8].

Experimental

Chemicals and instruments

Aspirin(acetylsalicylic) acid was purchased from Hyper Chem China. Anthracene purchased from Sigma–Aldrich, methanol for HPLC grid alpha China, Spectro fluorophotometer were measured on (RF-5301pc) Shimadzu, Electrical sensitive balanced Adam, and UV-Visible spectrophotometer (SPECORD 40, Analytic Jena GmbH).

Preparation of the samples

The compounds under study were dissolved in a precise volume of solvent before being used to make the solution, which was made by diluting various concentrations of the chemicals into the final solution [9]. The chemicals are made using the given equations:

$$\mathbf{W} = \frac{[\mathbf{M}]\times\mathbf{V}\times\mathbf{M.W}}{\mathbf{1000}} \qquad (2.1)$$

Where: W: material weight in (g), M.W.: molecular weight (g/ml), [M]: molar concentration (ml/L), V: the volume of solvent used to dissolve the material (ml) [10].
To dilute the solvent, use the following equation:

$$[\boldsymbol{M}]_1\boldsymbol{V_1} = [\boldsymbol{M}]_2\boldsymbol{V_2} \qquad (2.2)$$

Where [M] 1 is the concentration of the base, and [M] 2 is the concentration of the new solution. V1 is the volume of the solution before it was diluted, and V2 is the volume of the solution after it was diluted [11]. So, we prepare (1 µM) from aspirin and anthracene.

Absorption Measurements[12]

A spectrometer was used to determine the absorption spectra (SPECORD 40, Analytic Jena GmbH). UV-Visible spectrophotometer), as shown in Figure (1); this instrument operates in the visible and ultraviolet radiation ranges, with the following excitation lamps: The Deuterium lamp produced light with wavelengths ranging from (190 -480 nmm). Tungsten lamp: produces light with wavelengths ranging from 480 to 1100 nm, which can be utilized to cover the Ultraviolet-visible spectrum.

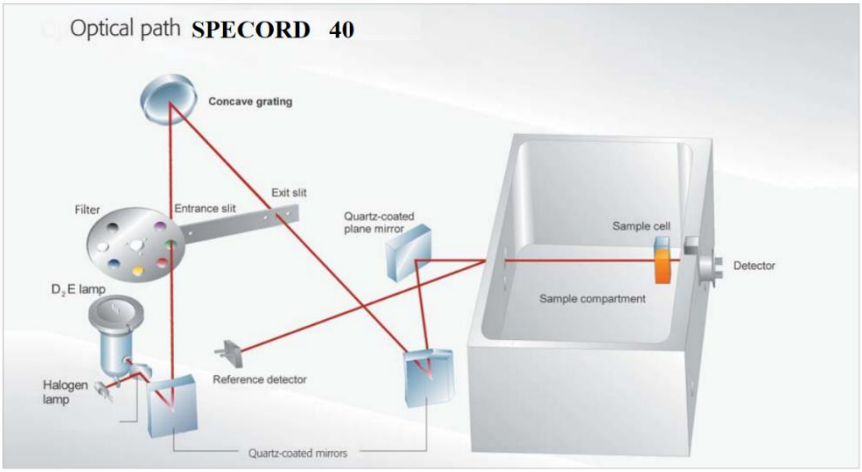

Fig. (1): Absorption patterns depicted by a single-beam spectrophotometer's schematic diagrams [12].

Fluorescence measurements[13]

A Spectro fluorophotometer (RF-5301pc Shimadzu) was used to quantify fluorescence emission from the samples generated in this figure (2). The samples were placed in a quartz cubic cell with a volume of (1 x 1 x 5) cm3 at a 90o angle to the incident beam. This optical geometry was chosen to limit the occurrence of self-absorption and eliminate the event of scattered light incident radiation. The computing equipment is machined, and it can work in the wavelength range (200-

900nm). Figure 3.3 shows a sketch of a fluorescence spectrometer, which you can add to the optical components displayed, a specialized computer controls instrument operation in the fluorescence spectrometer (excitation and emission wavelength, scan, monochromator dent width, sensing element parameter).

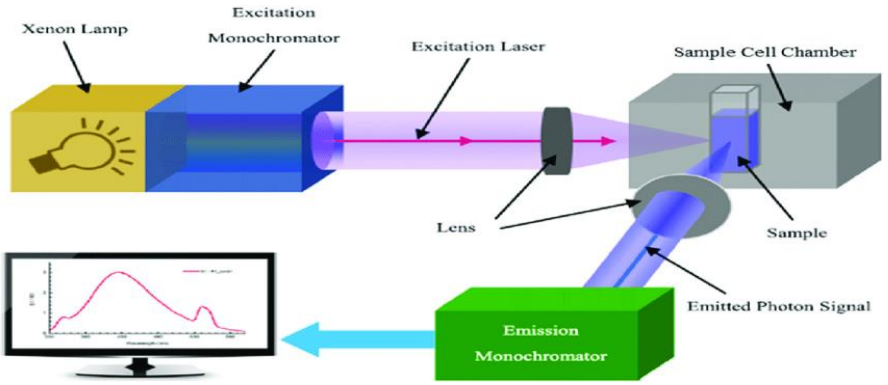

Fig. (2): Conventional right-angle fluorescence collecting block diagram [13]

Quantum yield

Quantum yield computation requires precise spectral correction. This method, which measures the number of emitted and absorbed photons, is called the absolute method for determining Emission Quantum Yield. Comparing to a reference standard with known emission quantum yield is another way for measuring quantum yield [14]. In our work use program a/e-UV-Vis-IR-Spectral-Analysis-Software to calculate the quantity Quantum Yield [15].

Results & Discussion

Absorption Measurements [16]

The absorption spectra of aspirin solutions dissolved in methanol were studied at room temperature with concentration (1 M) and highest peak spectral at wavelength (235 and 270 nm), as well as the absorption spectra of anthracene solutions dissolved in methanol with concentration (1 M) and highest peak spectral at wavelength (220, 245, 320, 340, 355, and 375 nm) in accordance with Beer-Lambert law (fig. 3 and 4).

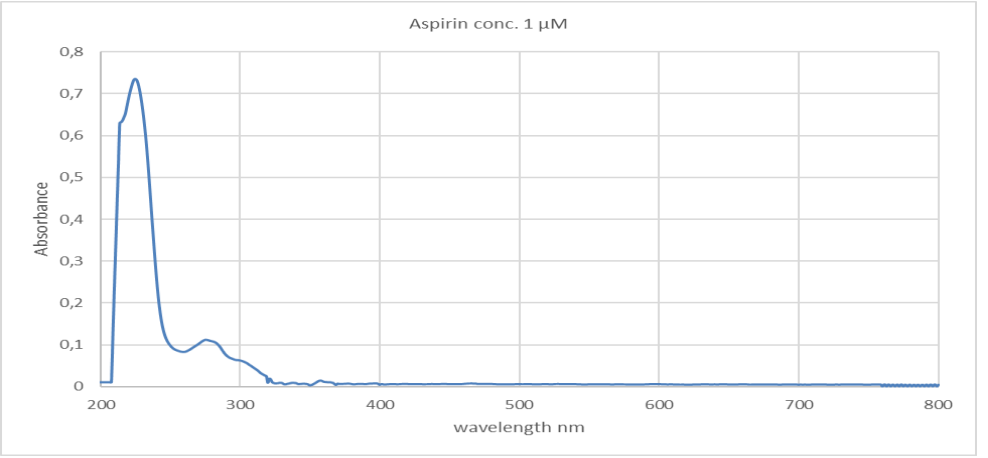

Fig. (3): At [1 M], the absorption spectra of aspirin dissolved in methanol are shown.

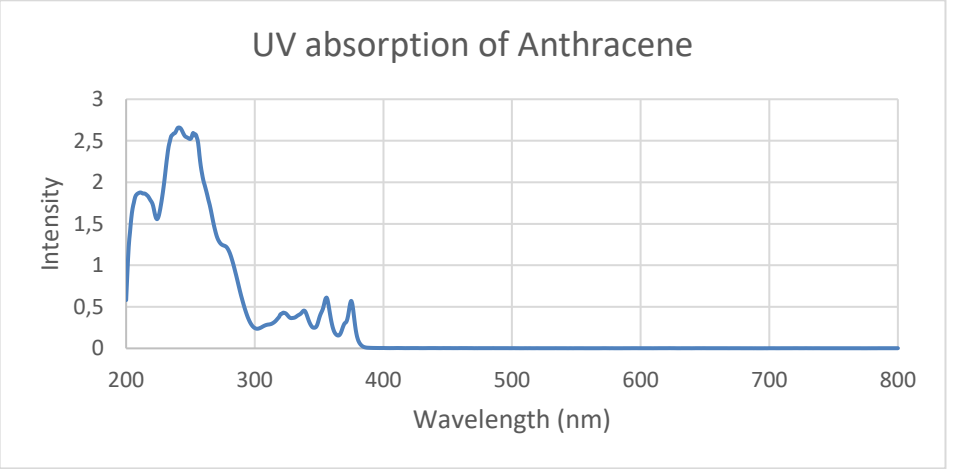

Fig. (4): At [1 M], the absorption spectra of Anthracene dissolved in methanol are shown.

The Fluorescence Spectra of aspirin [16]

At a concentration of [1 µM] and an excitation wavelength of 235 nm, the fluorescence spectra of aspirin molecules that had been dissolved in methanol were examined. In Fig.5 The fluorescence of a solution made from aspirin that had been dissolved in methanol at a concentration of [1 µM] showed that the following band appeared (0-0), and the emission wavelength was (400 nm).

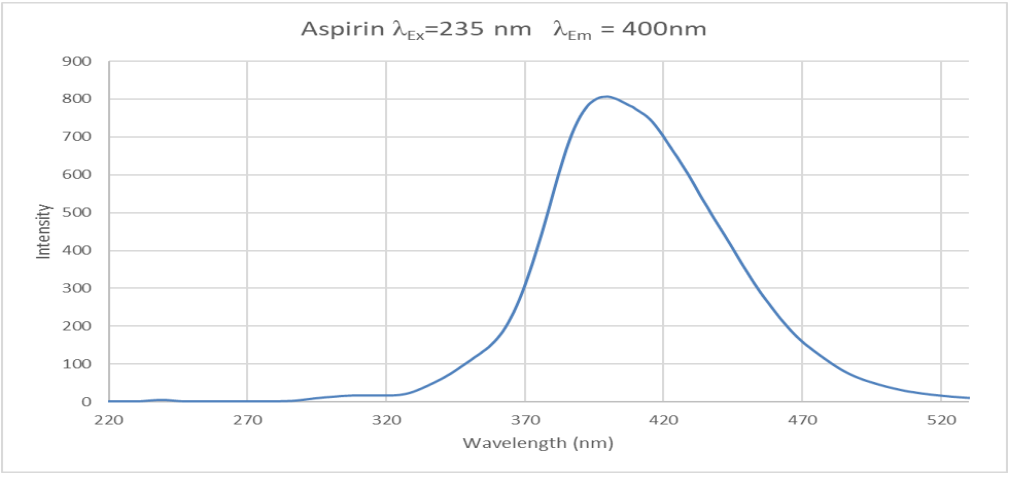

Fig. (5): Spectrum of fluorescence emitted by aspirin when dissolved in methanol at a concentration of [1 µM]

At a concentration of [1 µM] and at an excitation wavelength of (250 nm), the fluorescence spectra of anthracene molecules that had been dissolved in methanol were measured. In Fig. 6, there were visible bands (0-0) at emission wavelengths (380,400, 425, and 455nm) in the fluorescence of the Anthracene solution dissolved in methanol at concentration [1 mM].

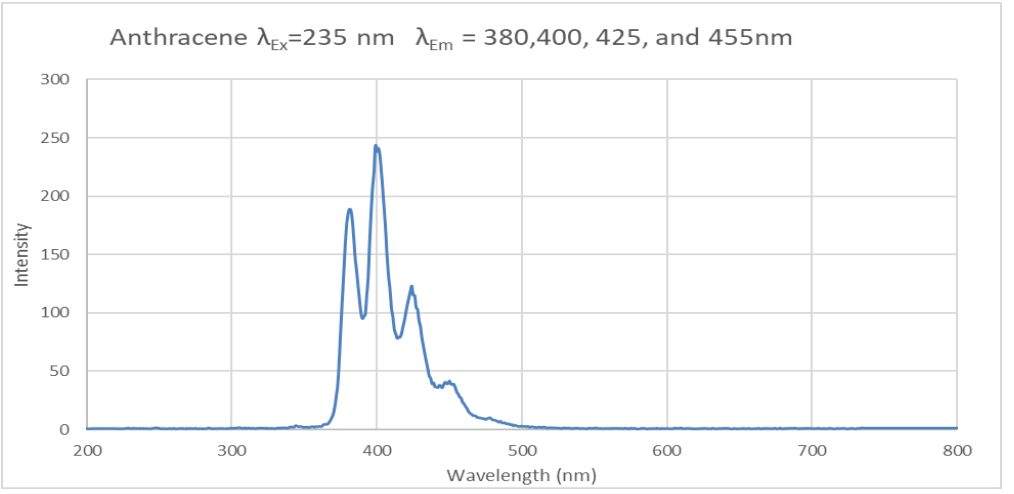

Fig. (6): Spectrum of fluorescence emitted by Anthracene when dissolved in methanol at a concentration of [1 µM].

Calculation of the quantum yield [15,17]

The a/e-UV-Vis-IR-Spectral-Analysis-Software arrived at the value QY=0.9987 when calculating the quantum yield for aspirin. According to the evidence presented in Figure 7, the spectrum of fluorescence emitted by the donor needs to overlap with the spectrum of reference (Ref.) absorption.

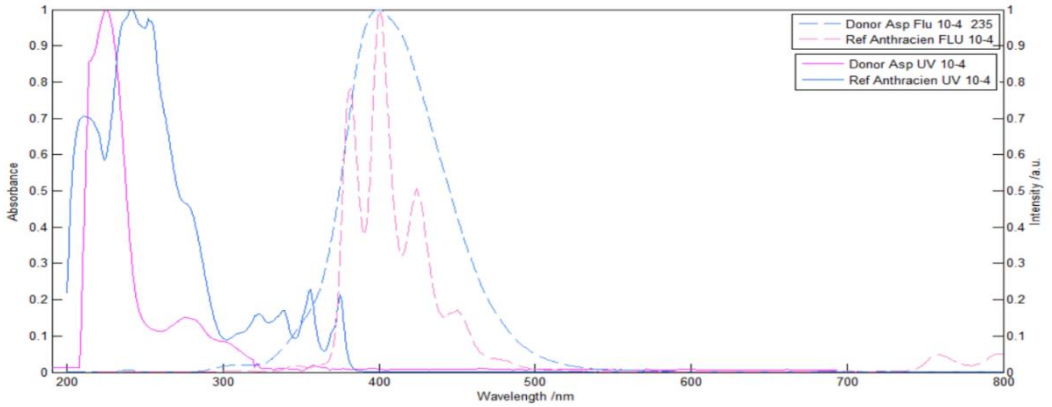

Fig. (7): Anthracene (Ref.) and aspirin (donor) absorption and fluorescence spectra in methanol at [1 μM]

Conclusions

In the present study, we study the spectra properties of absorption by spectrophotometer and the fluorescence by Spectro fluorophotometer from UV to visible range, for aspirin, we get that the aspirin exhibits a (λmax = 370–470 nanometer) fluorescence under ultraviolet (UV) wavelength .so this result led to use the aspirin as color violate sensor from (400-470 nanometer) due to the high quantum yield efficiency.

Declaration of Competing Interest

There are no conflicts of interest or personal ties that could have appeared to affect the work disclosed in this research, according to the authors of this paper

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