APPLICATION NOTE

DETERMINATION OF QUININE IN TONIC WATER SAMPLES USING FLUORESCENCE SPECTROSCOPY

INTRODUCTION

Fluorescence is the term used to describe the emission of cold light from a substance that occurs between two electronic states having the same nature. Consequently, the return to the ground state occurs rapidly with the emission rates from the substance being typically in the nanoseconds time range (10^{-9} s). Fluorescence is generally observed for a wide range of aromatic moelcules. Among typical fluorescent substances (fluorophores), quinine is one of the most remarkable fluorophores for its importance on the molecular fluorescence studies [1,2].

Quinie, see **Figure 1**, is an anti-malarial drug used as flavor in carbonated beverages, such as tonic water. In the 19th century, quinine mixed with carbonated water was highly consumed as a preventative measure for malaria disease [3,4].

However, due to its bitter taste, the traditional mixture with gin is used to make the tonic water taste more pleasant. When a glass of gin tonic is exposed to sunlight, a faint blue glow is frequently visible at the surface when observed in a right-angle configuration. The quinine in tonic water is excited by the ultraviolet light from the sun. Upon return to the ground state, quinine emits a blue light [2].

Keywords:

Fluorescence Spectroscopy;

LED Light Source;

SENSE Spectrometer;

Quinine;

Tonic Water;

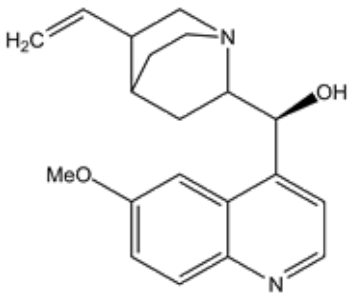

Figure 1 – Quinine molecular structure [2].

In this Application Note, we describe a method to determine the concentration of quinine in two water samples using our SENSE spectrometer. This method is based on the emission at the wavelenght maxima, around 450 nm.

MATERIALS & METHODS

Reagents

- Quinine [$(C_{20}H_{24}N_2O_2)_2.H_2SO_4.2H_2O$; MW ≈ 782.96 g/mol];
- H_2SO_4 (MW ≈ 98.08 g/mol; concentration: 0.05 M);
- Two commercially available tonic water samples;

Instruments and Accessories (Figure 2):

- LED Light Source;
- 365 nm LED Slide (excitation wavelength);
- Optical Fibers with 1000 µm of diameter (both 1 m long);
- Multipurpose Cuvette Holder (with signal enhancing mirrors);
- SENSE Spectrometer (Slit: 200 µm; Grating: 600 grooves/500 nm; Detector: Hamamatsu 2048 pixel);
- Two fluorescence quartz cuvettes with a pathlenght of 1 cm; SENSE Spectrometer (Slit: 200 µm; Grating: 600 grooves/500 nm; Detector: Hamamatsu 2048 pixel);

Figure 2 – LED Light source (1), SENSE spectrometer (2), and multipurpose cuvette holder (3) were used to determine the concentration of quinine in tonic water samples.

EXPERIMENTAL PROCEDURE

1. The quinine stock solution (100 mg/L) was prepared by weighting an accurate amount of quinine sulfate (10 mg) and diluted with a 0.05 M H_2SO_4 solution in a 100 mL volumetric flask;

2. A 10 mg/L standard was prepared by diluting the 100 mg/L stock solution with 0.05 M H_2SO_4 in a 100 mL volumetric flask;

3. A series of standard solutions of 0.8, 1.4, 2.0, 2.6. 3.2, 3.8, and 4.4 mg/L quinine sulfate were prepared by dilution with 0.05 M H_2SO_4 in a 100 mL volumetric flask;

4. Two different commercially available tonic water samples were analyzed by taking a small aliquot that was vigorously shaken in order to remove the dissolved carbon dioxide. From these degassed tonic water samples, 4 mL were collected and diluted to a final volume of 100 mL in 0.05 M H_2SO_4;

5. The fluorescence emission of standards and samples was measured and the background correction was carried out using a blank solution of 0.05 M H_2SO_4;

6. The instrument settings selected on the LightScan software are specified in **Table 1**;

Table 1 – Instrument settings used in fluorescence measurements.

Parameter	Value
Integration time (ms)	Variable
Average	4
Smoothing	2

RESULTS

The absorption and fluorescence spectra of a quinine sulfate dissolved in a 0.05 M H_2SO_4 are presented in **Figure 3**.

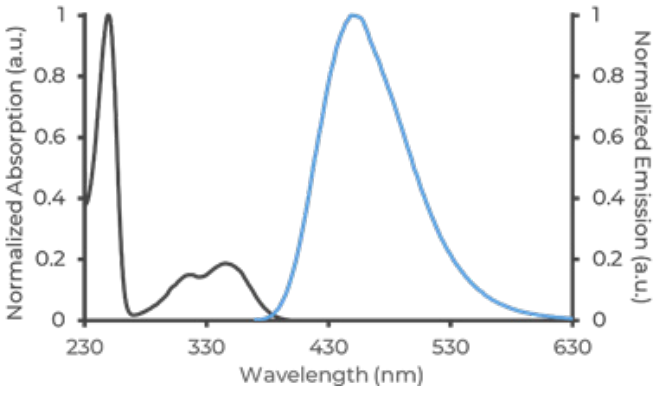

Figure 3 – Absorption (black line) and fluorescence (blue line) spectra of quinine sulfate in H_2SO_4 0.05 M.

The absorption spectrum of quinine sulfate shows a broad absorption band with two maxima between 273 and 400 nm. Below 273 nm is observed a strong absorption peak with a maximum around 250 nm.

Upon excitation at 365 nm, a fluorescence emission with a blue color is observed. In contrast with the absorption spectrum, quinine sulfate displays a broad fluorescence band with a maximum around 450 nm and no vibrational structure.

The calibration curve obtained for quinine sulfate is presented in **Figure 4**.

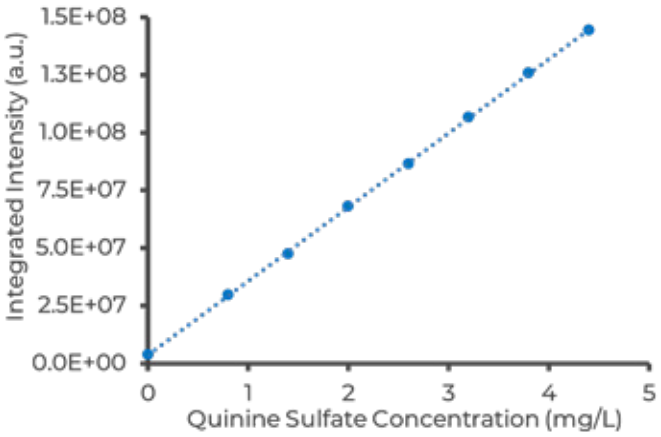

Figure 4 – Calibration curve of quinine sulfate in 0.05 M H_2SO_4. The fluorescence spectra were baseline corrected with 0.05 M H_2SO_4 solution and the integration time selected on the LightScan Software.

The integrated fluorescence intensity of quinine sulfate displays an excellent linear relation ($R^2 \approx 0.999$) in the range of 0.8 to 4.4 mg/L.

The concentration of quinine was determined by diluting 4 mL of the degassed tonic water samples in 100 mL of 0.05 M H_2SO_4, see **Table 2**.

Table 2 – Concentration of quinine in tonic water samples. Each determination was performed in triplicate and values were corrected for the 25-fold dilution factor.

Tonic Water Sample	Concentration (mg/L)
Sample 1	33.3±0.2
Sample 2	33.1±0.3

In order to correctly measure the amount of quinine in tonic water, a molar mass correction was performed (the calibration curve was performed with quinine sulfate which has a molar mass 2.41 times higher than that of quinine).

Therefore, upon correcting the concentration of quinine in both tonic water samples have similar values, which are around 33 mg/L.

The use of quinine as a flavour in beverages is currently limited by the United States Food and Drug Administration (FDA) to 83 mg/L, with most commercial tonic waters containing around 25 to 60 mg/L of quinine [3,5].

CONCLUSIONS

The use of fluorescence spectroscopy for detecting and measuring trace amounts of organic compounds is a major advantage over absorption spectroscopy. Our SENSE spectrometer in combination with our LED light source and Multipurpose Cuvette Holder allows for a simple and accurate determination of quinine in tonic water samples.

REFERENCES

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