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DESIGN CONCEPT: PORTABLE SPECTROSCOPY USING OPTICAL LIGHT PROPAGATION FOR RAPID LIQUID-BASED SENSING APPLICATION

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Abstract:

Ultraviolet-Visible (UV-VIS) spectroscopy is a technique used to measure the intensity of light absorbed after passing through a sample solution. UV-VIS spectroscopy analyses samples using light within the ultraviolet and visible wavelength ranges. Compared to other methods, this technique is non-invasive and less complex. However, current spectrometers are often bulky and not portable. Therefore, the objectives of this research are to design a portable Arduino-based spectroscopy system for liquid-based solutions and to integrate a motorised XY-axis into the proposed system. The spectroscopy setup includes a light source, Arduino, light sensor, stepper motor, gears, and pulleys. The XY-axis table was designed to adjust the optical light position, thereby improving measurement accuracy. Additionally, the dimensions of each component were identified, and the motorised structure of the XY-axis table was designed using 3D modelling. The proposed design is small, with dimensions of 16.5 cm (L) x 14 cm (W) x 13 cm (H). The experiment results on Kelulut honey showed that the average peak wavelength matched market spectroscopy values. The different XY-axis positions improved accuracy, making the system compact, portable, and motorised.

Keywords:

Spectroscopy; Portable; UV-VIS; Liquid-Based Solution; Optical Light Propagation

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Introduction

In the 1970s, the development of Light-Emitting Diode (LED)-based spectroscopies was introduced. This method aimed to create more advanced and refined spectroscopies, which are now widely available in many commercial analytical devices. A major drawback of the spectroscopies currently available on the market is their bulky and non-portable design (Benjamin O. Asamoah, Emilia Uurasjärvi, Jukka Räty, Arto Koistinen, Matthieu Roussey and Kai-Erik Peiponen, 2021). In addition, the lack of portability reduces the efficiency of workflows in research and development laboratories. Therefore, the bulkiness of current spectroscopies makes these processes more complicated, necessitating additional time and effort for setup, calibration, and relocation (Chai, 2020) (Mikhailenko, 2023). Hence, this research aims to design a portable Arduino-based Ultraviolet-Visible (UV-VIS) spectroscopy system that uses an optical light sensor for liquid sample identification and incorporates a motorised XY-axis for the light source. Spectroscopy is a method used to study the characteristics of light and other electromagnetic radiation, often to determine a substance's composition, structure, or concentration (Halim, 2023). It measures the intensity of light at various wavelengths after it interacts with a sample. Depending on the electromagnetic spectrum range and the detection technique, there are several forms of spectroscopy. For instance, Fourier Transform Infrared (FTIR) spectroscopy is commonly used to determine the chemical bonds within a molecule by measuring the amount of infrared light absorbed (Pérez-Cova, 2021). UV-VIS spectroscopy measures light absorption from the visible to the ultraviolet range from 200 nm to 800 nm (Batubara, 2022). It is used to determine chemical concentrations and study electronic transitions in molecules.

This research used UV-VIS spectroscopy because it is non-invasive and inexpensive, unlike other types of electromagnetic radiation (Quevedo, 2021) (Wieduwilt, 2022) (Cazzaniga, 2021). For example, Neshasteh-Riz *et al.* (Neshasteh-Riz, 2018) used X-rays and gamma rays to study hyperthermia. However, X-rays, gamma rays, Cobalt-60, and TLD-100 are invasive, damaging, or killing cells, and their devices are bulky and not portable (Xiang, 2021) (Park, 2022). Modern spectroscopies often overlook portability. FTIR spectroscopy, commonly used to identify organic materials (Dutta, 2017), is bulky and not portable (Chai, 2020). Additionally, the light source in FTIR devices is fixed and cannot be moved. Even though this proposal uses the UV-VIS spectroscopy technique, current devices on the market have the same drawbacks: they are bulky and non-portable (Park H. Y., 2021). This bulkiness makes UV-VIS spectroscopy impractical for field analysis (Mikhailenko, 2023). Additionally, UV-VIS spectroscopy has limited sensitivity, especially at deficient concentrations (Nandiyanto, 2018). Note that the light source is fixed and immovable.

A portable UV-VIS spectrometer can be made using Arduino, as the ATMega328P is one of the most flexible and versatile microprocessors available today. Using an LED as the light source, the UV-VIS spectrum can be achieved. Nandiyanto *et al.* (Nandiyanto, 2018) created a simple, rapid, and portable Arduino-based spectroscopy using a white LED to analyse solution concentration. Their design resulted in a compact spectrometer with dimensions of 20 × 13 × 15 mm (Nandiyanto, 2018). However, this spectroscopy is larger than the proposed design, and its light source is fixed. In contrast, Poh *et al.* created a smaller, Arduino-based spectrometer with Bluetooth feature to transfer data directly to smartphones. Their 2-in-1 UV-VIS spectroscopy device measures 105 × 90 × 140 mm and is controlled by a compact Arduino Nano (Poh, 2021). Nevertheless, this spectroscopy lacks the ability to adjust the light source position, which limits sample analysis. Yuniati *et al.* (Yuniati, 2019) designed a UV-VIS

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spectrometer with a stepper motor to change the spectrum color. However, their spectrometer is larger than the proposed design, and the light source position is fixed, with the stepper motor only changing the spectrum color, not the light source position [18]. Thus, this paper introduces a device concept that improves the size, portability, and light propagation studies with a motorised XY-axis. The device measures 16.5 cm (L) x 14 cm (W) x 13 cm (H) and weighs under 1 kg. It is handheld for better portability and is entirely black to reduce noise.

This paper is organised as follows: the methodology section describes the device's fundamental concept, hardware design, and process flowchart. The results section presents the preliminary findings of the proposed spectroscopy, and the conclusion section summarises the study.

Methodology

Fundamental Concept of Spectroscopy

Optical Light Spectrum

Light is the range of electromagnetic spectrum frequencies that are visible to human eyes (Duncan, 2012). When light of a given wavelength is transmitted through the sample through a light beam, each substance in the solution either absorbs or transmits the light of that wavelength. Electric and magnetic fields are force fields that surround charged particles and have an impact on nearby charged particles, oscillate, or vibrate, resulting in the waves that precede light. The electromagnetic spectrum is a wide range of frequencies or wavelengths of electromagnetic waves (Zwinkels, 2015). Figure 1 shows the electromagnetic spectrum. From Figure 3, it is pretty evident that the visible spectrum is only a small portion of the electromagnetic spectrum. The range of frequencies between 1 Hz and 1026 Hz that the human eye can perceive is quite narrow. The frequency range of visible light is very high, i.e., from 5 x 1014 to 7.5 x 1014 Hz, and their wavelength is from 400 nm to 800 nm. Each distinct frequency or wavelength of visible light results in a slightly different colour than normal human eyes would see. At roughly 800 nm, dark red has the longest wavelength humans can see, and humans can perceive wavelengths as short as 400 nm in deep blue or violet.

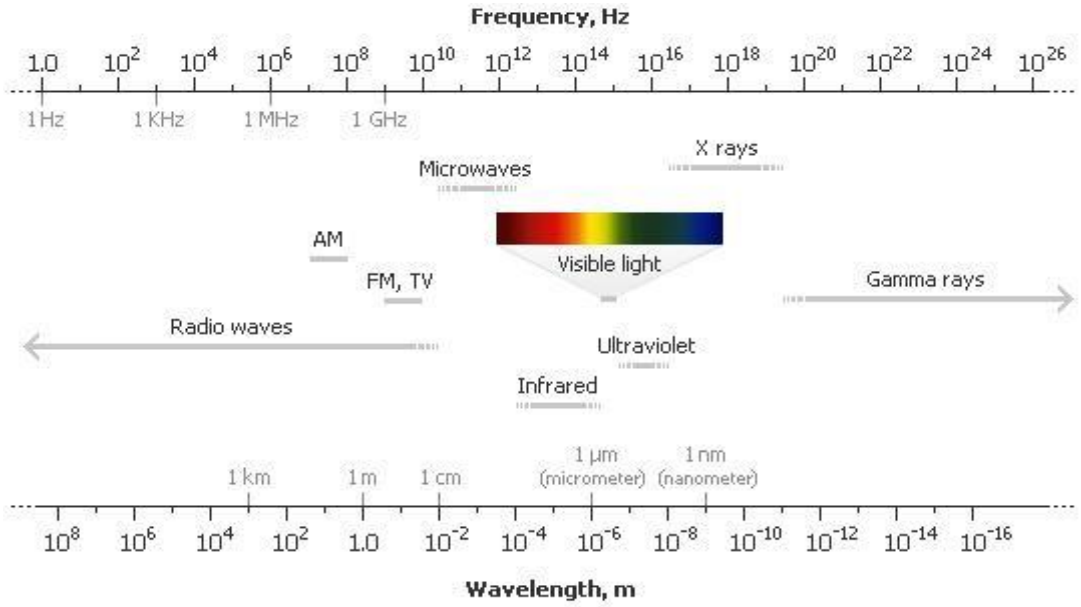

Figure 1. Electromagnetic spectrum [14]

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Optical light propagation is the motion of light through various mediums or across space. It includes several physical concepts that determine how light behaves in various conditions and explains how it travels from one place to another. Light travels through various mediums during the process of its dispersion. Note that light changes direction when it transitions across objects because it changes in speed as it moves through various materials. This bending of light is referred to as refraction. It also includes diffraction, the bending of light around barriers, and reflection, the bouncing off surfaces. When light waves merge, interference happens, creating either constructive or destructive patterns. Materials could scatter or absorb light, and the orientation of light wave oscillations is referred to as polarisation. These characteristics are essential in optics and other technologies because they help humans comprehend how light reacts with its surroundings.

The visible spectrum is just a tiny portion of the electromagnetic spectrum, as is readily apparent. The human eye can only detect a relatively small range of frequencies, from 1 Hz to 10^{26} Hz (Horning, 2019). Visible light has a relatively wide frequency range (5 x 10^{14} to 7.5 x 10^{14} Hz) and a wavelength (400–800 nm). A small variation in colour is perceived by the human eye at each unique frequency or wavelength of visible light. The longest wavelength humans can see is about 700 nm in dark red, whereas humans can also detect wavelengths as short as 400 nm in deep blue or violet. The normal definition of darkness includes the absence of light. However, darkness should be interpreted as the absence of electromagnetic waves in the visible light spectrum (Poh, 2021).

Optical Light Propagation Method: Absorbance And Transmittance

Figure 2 illustrates the emission of optical light parameters used in this proposed concept. This research examines how optical light propagation interacts with liquid-based solutions, focusing on Transmittance (T) and absorbance. The method relies on Beer-Lambert's law, which connects substance concentration to light absorption. Consequently, absorption occurs when a molecule absorbs photons from an excitation light source without emitting any. Beer-Lambert's law states that absorbance (A) is proportional to concentration (c) and path length (l). For example, a higher concentration or longer path length increases absorbance. This principle is fundamental in techniques such as UV-VIS spectroscopy. Mathematically:

$$A = \varepsilon c l, \tag{1}$$

where ε is the molar absorptivity or extinction coefficient, which represents the substance's ability to absorb light at a specific wavelength, the path length of light *l*, and the concentration of the analyte c (Oshina, 2021), the law applies if the sample adheres to ideal Beer-Lambert conditions: dilute, uniform absorption, and no significant interactions. Beer-Lambert's law quantifies substance concentration using spectroscopy by measuring light absorbance at specific wavelengths. This relationship shows that higher concentrations absorb more light, as the law's linear equation demonstrated. For example, solutions with higher concentrations exhibit increased absorbance.

On the other hand, T is the fraction of light that passes through a sample and is related to absorbance. The T formula shows how concentration and path length affect light transmission. Higher concentrations or longer path lengths reduce T, indicating more light absorption. This principle helps quantify absorbing species in spectroscopy. The formula for absorbance in terms of T can be derived from these equations:

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$$A = -log\ T = -log \frac{I}{I_o}, \quad (1)$$

where I is the irradiance of the beam emerging from the sample, and I_o represents the irradiance of the beam entering the sample (Sankaran, 2014). Spectroscopy can be expensive, but it can be built cheaply with Arduino. A Light-Dependent Resistor (LDR), or photocell, detects changes in light. In turbid solutions, the sensor registers low light levels, resulting in a decreased output voltage (Park H. Y., 2021). This voltage can replace the variables in Equation (2) to calculate absorbance.

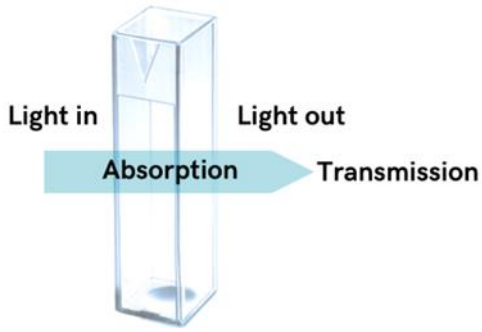

Figure 2. Emission of Optical Light Parameters

Cuvette: Z Dimension

A cuvette is a small, clear container used for liquid samples in spectroscopy. Made from quartz, glass, or plastic, it ensures a precise light path length and is standardised to fit optical devices for accurate measurements. Cuvettes come in various shapes and sizes to accommodate different sample volumes. For example, quartz cuvettes are preferred in UV spectroscopy for their high transmission, enhancing measurement accuracy and repeatability.

The z-dimension of a cuvette is the height from the base to the centre of the optical path, which is crucial for precise absorbance measurements. An incorrect z-dimension can misalign the light path and affect accuracy. Standard cuvettes typically have a z-dimension of 8.5 mm or 15 mm. Therefore, maintaining the correct z-dimension is vital for consistency and reliable results in spectroscopy. Different cuvette shapes affect the z-dimension. Longer z-dimensions in high-path length cuvettes increase sensitivity for low-concentration samples. In contrast, shorter z-dimensions in low-path length cuvettes are used for high-concentration samples, reducing absorbance. Cylindrical cuvettes may have variable z-dimensions optimised for specific light paths. Hence, knowing the correct z-dimension ensures accurate alignment and measurement, enhancing precision and reliability in experiments.

Proposed Device Design

Hardware 3D Design

The hardware 3D concept design is illustrated in Figure 3 below. TinkerCAD software was used to create the 3D drawing. The proposed design was compact to fit the dimensions of all components. It includes the basic arrangement of a spectroscopy system, which consists of an optical light source, slit, detector, and display system. The light source section consists of a funnel, bolt stand, bearing, and bolt. The funnel contains a Red-Green-Blue (RGB) LED light

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that directs the light source to ensure it travels in a straight, focused path without scattering. In this design, the funnel and the cuvette were not attached to each other. The funnel and cuvette were placed close together to improve the accuracy of measurements for the cuvette, funnel, bolt support, bearing, and bolts. The bolt support holds the bolt in place, which secures the bearing. The bearing supports the light source section on the X-axis and allows it to move. The X-axis moves the light source along its direction and uses a bearing to keep it stable and aligned during analysis. Correspondingly, the Y-axis moves the light source along its direction and supports all components on both axes. It is permanently attached to the project base for added strength and stability. The Arduino Mega was used in this research and programmed with Arduino IDE. The device was 3D-printed with black PLA filament to reduce light reflection and scattering.

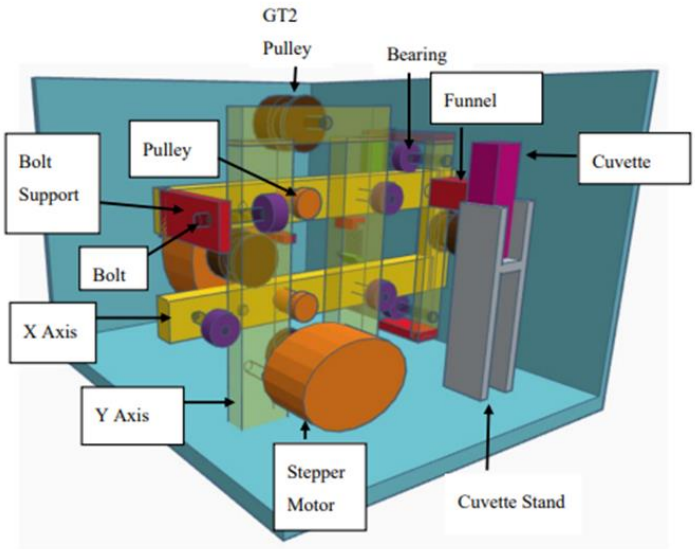

Figure 3. 3D Hardware Design

Proposed Design Process Flowchart

Figure 4 illustrates the device process flowchart. In the first step, an LED light source was used where the light diffracted across the UV-VIS spectrum. The concept of optical light propagation was discussed in Section 2.1.2. Subsequently, the sensor measures the absorbance after the light passes through the sample solution. Measurement results were displayed on both the LCD and the Serial Monitor of the Arduino IDE. For example, absorbance values are recorded and shown on these displays. The stepper motor moves the cuvette through the XY-axis to various positions. The motor positions the cuvette at the top right, top left, bottom left, and bottom right. The process includes rotating the cuvette around the X-axis at specific angles. These positions were stored in an array during the coding process. Each completed position is marked in the array. The iteration process is complete once all the positions in the array are fulfilled. This results in five absorption measurements at different light source positions. Finally, the light source returns to the center, completing the process. The targeted particle in the cuvette might not always be in the center of the cuvette. Moreover, the particle might even move in the liquid sample. The whole liquid sample in the cuvette can be analysed by changing the XY optical light position.

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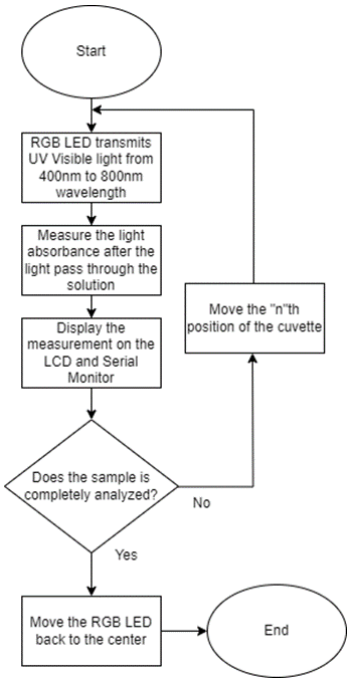

Figure 4. Device Process Flowchart

Preliminary Results

Pure Kelulut honey was used as the initial sample to test the proposed device. As illustrated in Figure 5, measurements were taken at the Center (CT), Top Right (TR), Top Left (TL), Bottom Left (BL), and Bottom Right (BR). The X-axis represents the UV-VIS wavelength range from 380 nm to 780 nm, while the Y-axis shows absorbance units (a.u). Each position displayed slightly different peak absorbance values, indicating variations in the sample's absorbance at different locations. The peak absorbance values for CT, TR, TL, BL, and BR were 1019 a.u, 1017 a.u, 1017 a.u, 1018 a.u, and 1017 a.u, respectively, with corresponding wavelengths of 707 nm, 708 nm, 704 nm, 705 nm, and 706 nm.

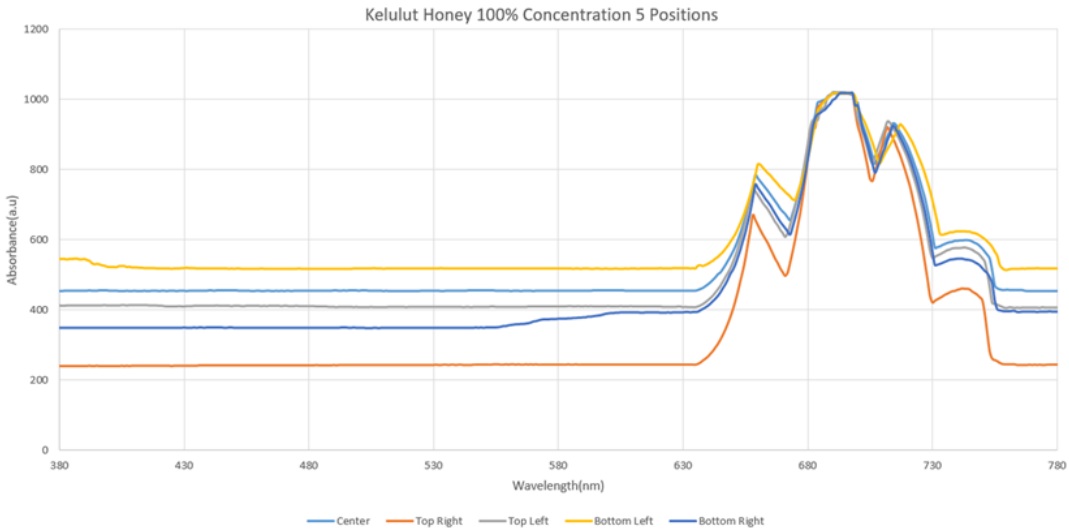

Figure 5. Absorbance vs. Wavelength Graph for Kelulut Honey at five Different XY Positions

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Based on these values, an average of the five measurements was plotted in Figure 6, which indicates the average absorbance unit vs. wavelength graph. However, some noise was recorded at three additional lower peaks, likely due to the low-cost sensor used. Compared to the research in (Sankaran, Introduction to the electromagnetic spectrum, 2014) using a commercial spectrometer, our device showed a wavelength peak margin difference of around ±5 nm, demonstrating that the proposed spectroscopy is reliable, as the results closely align with those of a commercial system. Additionally, the use of different XY-axis positions improved measurement accuracy. Overall, these preliminary results suggest that the proposed device performs as expected.

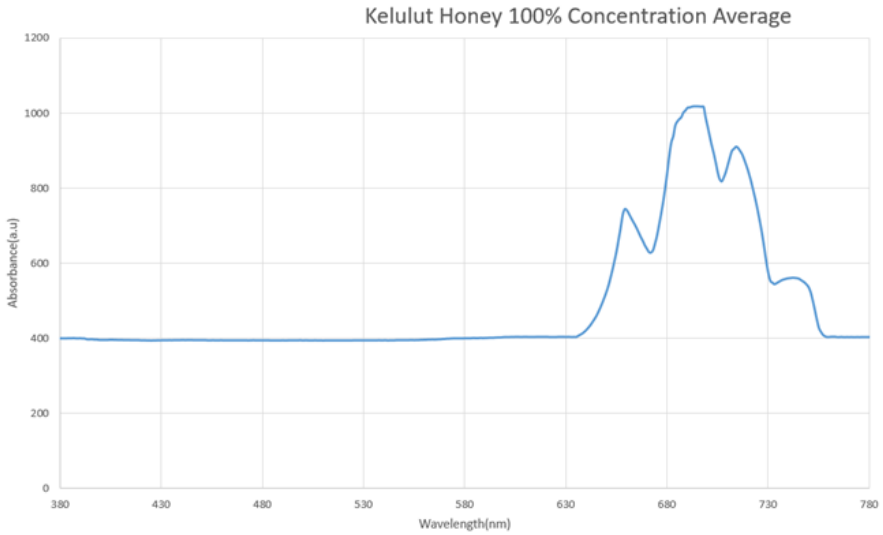

Figure 6. Average Absorbance vs. Wavelength Graph for Pure Kelulut Honey

Conclusions

The development of the proposed non-invasive and portable spectroscopy represents a significant advancement in analytical devices. This innovative technology offers numerous benefits and opportunities across various industries. Therefore, eliminating the invasiveness of traditional methods preserves the integrity of liquid-based samples, allowing for further analysis and potential reuse. This minimises waste and maximises resource efficiency. The device's portability enables on-site analysis, fieldwork, and point-of-care applications, revolutionising sample identification and analysis. Its compact design and ease of use enhance integration into laboratory workflows, boosting efficiency and productivity. This technology holds great promise for industries such as pharmaceuticals, environmental monitoring, quality control, and research and development.

Furthermore, the proposed non-invasive and portable spectroscopy aligns with sustainable development principles. It contributes to sustainable infrastructure by promoting technological innovation and reducing the environmental impact associated with invasive analysis methods. This advancement makes analysis more accessible and efficient, paving the way for improved decision-making, quality assurance, and research outcomes. Other than that, the device's accuracy is high and meets expected results, although some noise may still be present as a low-cost sensor was used for this device.

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In summary, non-invasive and portable spectroscopy is a big breakthrough in analytical technology. It can analyse liquid samples accurately without being invasive and is easy to use and portable. This technology in everyday work can make processes more efficient, reduce waste, and support sustainability. The future looks bright for this technology, with more improvements expected to meet new needs and advance both research and industry applications.

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