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Portable Spectroscopy with Movable Light Source for Rapid Liquid Sensing via Optical Light Propagation

Muhammad Nurullah Waliyullah Mohamed Nazli[1], Irneza Ismail[1,*]

[1] Faculty of Engineering and Built Environment Universiti Sains Islam Malaysia (USIM), Nilai, Negeri Sembilan, Malaysia

ABSTRACT

Ultraviolet-Visible (UV-VIS) spectroscopy measures light absorption intensity in a sample solution. This technique operates within the UV-Visible wavelength range. UV-VIS spectroscopy analyses samples using light within the ultraviolet and visible wavelength ranges. This method is non-invasive and simpler than other techniques. However, current spectrometers are often less sensitive to low concentration samples, bulky and not portable. Therefore, the aim of this research is to incorporate a motorized XY axis into the system as well as focusing on designing a portable Arduino-based spectroscopy system for liquid solutions. The spectroscopy setup includes stepper motors, gears, pulleys, an XY axis system, light source, Arduino and light sensor. The XY axis table is designed to adjust the optical light's position which enhances the sensor's sensitivity. The dimensions of each component are measured. A 3D modelling is used to design the motorized XY axis table. The proposed design is small, with dimensions of 16.5 cm (L) x 14 cm (W) x 13 cm (H). The reliability of the proposed spectroscopy system is evaluated using Kelulut Honey. The obtained results are then analyzed. In conclusion, the proposed spectroscopy system features a motorized XY mechanism, compact and portable.

Keywords: *Spectroscopy; portable; UV-VIS; liquid-based solution; optical light propagation*

1. Introduction

Spectroscopies are commonly used in commercial analytical devices. These technologies are further enhanced in 1970s by implying LED-based features. This innovation aimed to enhance spectroscopic techniques. However, major limitations of current spectroscopic instruments are their low sensitivity, bulky and lack portability [1]. The light source in most spectrometers remains fixed, resulting in limited sensitivity when analyzing low concentration sample. The lack of portability decreases workflow efficiency in research and development laboratories. The bulkiness of current spectroscopic devices complicates these processes. This design leads to increased time and effort for setup and calibration. Additionally, relocating these devices is more challenging [2,3]. To address these challenges, a motorized XY axis for the light source in a spectroscopy system in which will enhance sensitivity. Additionally, a portable Arduino-based UV-VIS spectroscopy system will be designed. This system will utilize an optical light sensor for identifying liquid samples. Spectroscopy is a technique for analyzing light and other electromagnetic radiation. It helps determine the composition, structure, or concentration of a substance [4]. It measures transmittance of transmitted electromagnetic radiation after passing through the sample across different wavelengths after

* *Corresponding author.*
E-mail address: dr.irneza@usim.edu.my

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interacting with a sample. Various forms of spectroscopy exist, depending on the electromagnetic range and detection methods used. For example, Fourier Transform Infrared (FTIR) spectroscopy is commonly used to determine the chemical bonds within a molecule by measuring the amount of infrared light absorbed. UV-VIS spectroscopy measures light absorption from the visible to the ultraviolet range [5]. It is used to determine chemical concentrations and study electronic transitions in molecules. UV-VIS wavelength ranges from 200nm to 800nm [6,7]. UV-VIS also can analyze solid form sample, as long as light still can pass through the sample.

This research utilized UV-VIS spectroscopy due to its non-invasive nature towards samples. It is also cost-effective compared to other electromagnetic radiation methods [8,9]. For instance, X-rays and gamma rays are used to study hyperthermia. X-rays are also used in mammography method to identify breast cancer [22]. However, X-rays, gamma rays, Cobalt-60, and TLD-100 are invasive towards samples where it damages or worse, killing the cells. Their devices are also bulky and not portable [10,11]. Modern spectroscopies often overlook the value of portability. FTIR spectroscopy, commonly used to identify organic materials, is bulky and not portable [2,12]. Additionally, the light source in FTIR devices is fixed and cannot be moved. Even though this research also uses the UV-VIS spectroscopy technique, current devices on the market have the same drawbacks: they are bulky and non-portable [13]. This bulkiness makes UV-VIS spectroscopy impractical for field analysis [3]. Additionally, UV-VIS spectroscopy has limited sensitivity, especially at very low concentrations, the light source is fixed and immovable [14].

A portable UV-VIS spectrometer can be made using Arduino, as the ATMega328P is one of the most flexible and versatile microprocessors available today. By using an LED as the light source, the UV-VIS spectrum can be achieved. A simple, rapid, and portable Arduino-based spectroscopy using a white LED to analyze solution concentration. Their design resulted in a compact spectrometer with dimensions of 20 × 13 × 15 mm [15]. However, this spectroscopy is larger than the proposed design, and its light source is fixed. In contrast, a smaller, Arduino-based spectrometer with Bluetooth feature to transfer data directly to smartphones also created another researcher [16]. Their 2-in-1 UV-VIS spectroscopy device measures 105 × 90 × 140 mm and is controlled by a compact Arduino Nano. Nevertheless, this spectroscopy lacks the ability to adjust the light source position, which limits the sensitivity during the sample analysis. A UV-VIS spectrometer with a stepper motor to change the spectrum color is invented as another way of improving spectroscopy. However, their spectrometer is bulkier than the proposed design, and the light source position is fixed as the utilization of stepper motor is only for changing the spectrum color, not the light source position [17]. Thus, this paper introduces a device concept that improves size, portability, and light propagation studies with a motorized XY axis. The device measures 16.5 cm (L) x 14 cm (W) x 13 cm (H) and weighs under 1 kg. It has handheld feature for better portability and is entirely black to reduce noise.

2. Methodology

2.1 Device Design

2.1.1 Proposed 3D design

TinkerCAD software is used to create the 3D drawing. The proposed design is 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 funnel, bolt stand, bearing and bolt. The funnel contains a Red-Green-Blue (RGB) LED light that directs the light source to ensure it travels in a straight, focused path without scattering. In this design, the funnel and the cuvette are not attached to each other. The funnel and cuvette are 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 bearing to keep it stable and aligned during analysis. 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.

Figure 1 and Figure 2 shows the proposed spectrometer. With dimension of 16.5 cm (L) x 14 cm (W) x 13 cm (H), this spectrometer is portable. With weight below 1kg, it can easily be relocated. Arduino Mega is used as it has more pins. Arduino Mega is programmed using the free software, Arduino IDE. The proposed device is printed using 3D printer, using PLA filament as the main materials. Black colored PLA filament is used to reduce light reflection and scattering inside the proposed device. The side walls of the spectrometer are made of acrylic to avoid external light intervention and to reduce light scattering.

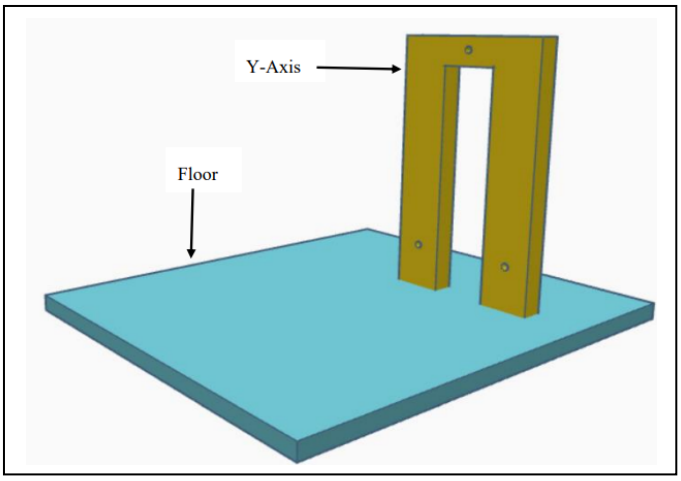

Fig. 1. Y axis section of the proposed spectroscopy

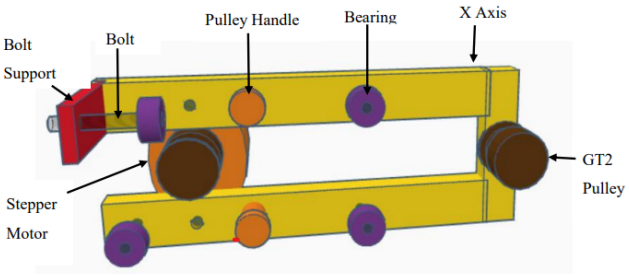

Fig. 2. X axis section of the proposed spectroscopy

2.1.2 Proposed design flowchart

Figure 3 illustrates device process flowchart. In the first step, LED light source is used where the light diffracts across the UV-VIS spectrum. The concept of optical light propagation is discussed under Device Concept section. The sensor then measures the absorbance after the light passes through the sample solution. Measurement results are 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 Y-Z 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 are stored in an array in coding process. For each position completed, the position will be marked in the array. When all the positions in the array is

fulfilled, then the iteration process is completed. 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. By changing the optical light position, the whole liquid sample in the cuvette can be analyzed hence the sensitivity of the device is improved.

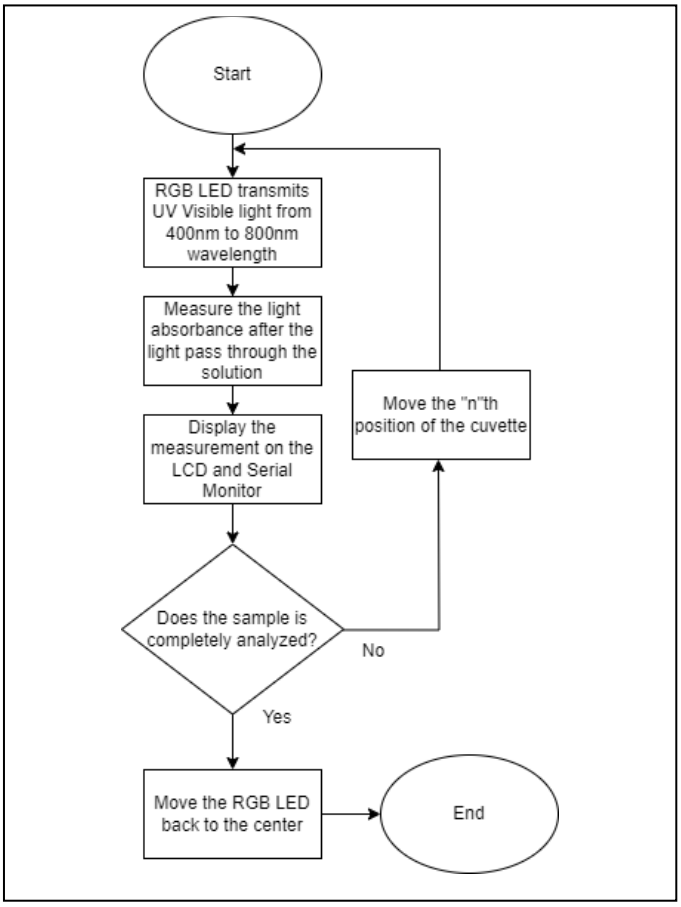

Fig. 3. Design process flow chart

2.2 Device Concept

2.2.1 Fundamental concept of spectroscopy

Light is the electromagnetic wave that travels in the range of electromagnetic spectrum frequencies that are visible to human eyes [18]. 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, which 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 [19]. Figure 4 shows the electromagnetic spectrum. From Figure 4, 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 range of frequencies between 1 Hz and 10^{26} Hz that the human eye can perceive is quite narrow. The frequency range of visible light is very high i.e. from 5 x 10^{14} to 7.5 x 10^{14} Hz and their wavelength is from 400 nanometers to 800 nanometers. Each distinct frequency or wavelength of visible light results in a little different color that normal human eyes would see. Dark red, at roughly 800 nm, has

the longest wavelength that humans can see, and humans can perceive wavelengths as short as 400 nm in deep blue or violet.

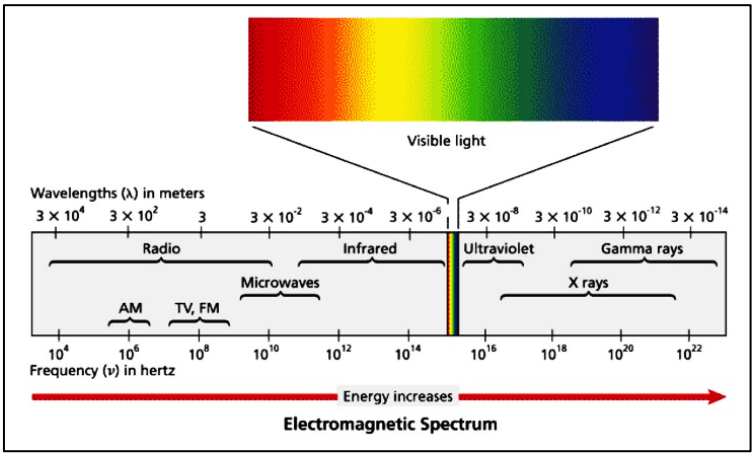

Fig. 4. Electromagnetic spectrum [20]

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 light travels from one place to another. Light travels through various mediums during the process of its dispersion. 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 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 polarization. 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 it is readily apparent. The human eye can only detect a relatively small range of frequencies, from 1 Hz to 10^{26} Hz [20]. Visible light has a relatively wide frequency range (5 x 10^{14} to 7.5 x 10^{14} Hz) and a wavelength (400–800 nanometers). A small variation in color is perceived by the human eye at each unique frequency or wavelength of visible light. The longest wavelength that 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. Normal definition of darkness is the absence of light. However, darkness should be interpreted as the absence of electromagnetic waves in the visible light spectrum [21].

2.2.2 Principle of optical light propagation: absorbance and transmittance

Figure 5 shows 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 and absorbance. The method relies on Beer-Lambert's law, which connects substance concentration to light absorption. Absorption occurs when a molecule absorbs photons from an excitation light source without emitting any light. 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.

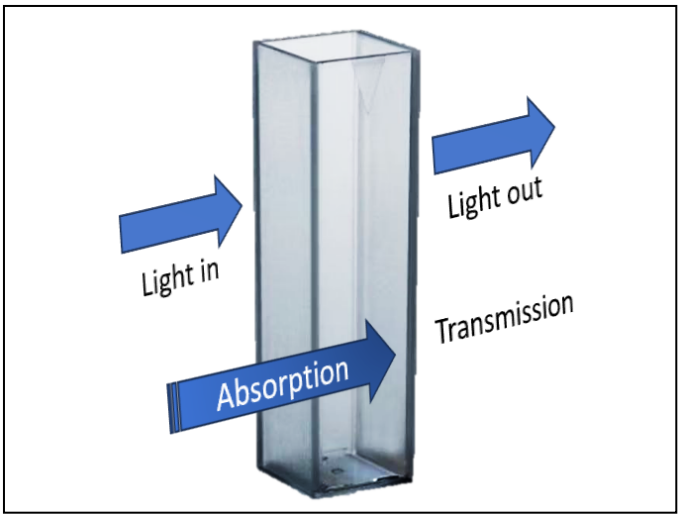

Fig. 5. Emission of optical light parameters

This principle is fundamental in techniques such as UV-VIS spectroscopy. Mathematically,

$$A = \varepsilon cl \tag{1}$$

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* [23]. 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 demonstrated by the law's linear equation. For example, solutions with higher concentrations exhibit increased absorbance.

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

$$A = -log\ T = -log \frac{I}{I_{\circ}} \tag{2}$$

where *I* is the irradiance of the beam emerging the sample and I_o represents the irradiance of the beam entering the sample [24]. 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 [15]. This voltage can replace the variables in Eq. (2) to calculate absorbance.

2.2.3 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 standardized to fit optical devices for accurate measurements. Cuvettes come in various shapes and sizes to accommodate different sample volumes. Quartz cuvettes, for example, 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. 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, while shorter z-dimensions in low path length cuvettes are used for high-concentration samples, reducing absorbance. Cylindrical cuvettes may have variable z-dimensions optimized for specific light paths. Knowing the correct z-dimension ensures accurate alignment and measurement, enhancing precision and reliability in experiments.

3. Results

3.1 Results and Discussion

To test the proposed device, supermarket honey is used as the first sample. The X axis represents the wavelength range while the Y axis represents the absorbance unit (a.u). The wavelength range of X axis starts from 380nm to 780nm as it indicates the wavelength range of UV-VIS. For each concentration, five measurements are taken at different positions: center (CT), top right (TR), top left (TL), bottom left (BL), and bottom right (BR). All 5 measurements have different peak absorbance considering there might be difference in the sample's concentration at different position as shown in Figure 6. The peak absorbances for CT, TR, TL, BL and BR are 625a.u at 555nm, 599a.u at 562nm, 564a.u at 562nm, 631a.u at 559nm, and 502a.u at 559nm, respectively. From the differences in absorbance value measured at each position, the concentration of supermarket honey at CT is higher than the concentration of supermarket honey at BL and concentration at BL is higher than the concentration at TR, TL and BR. The average of these measurements is plotted.

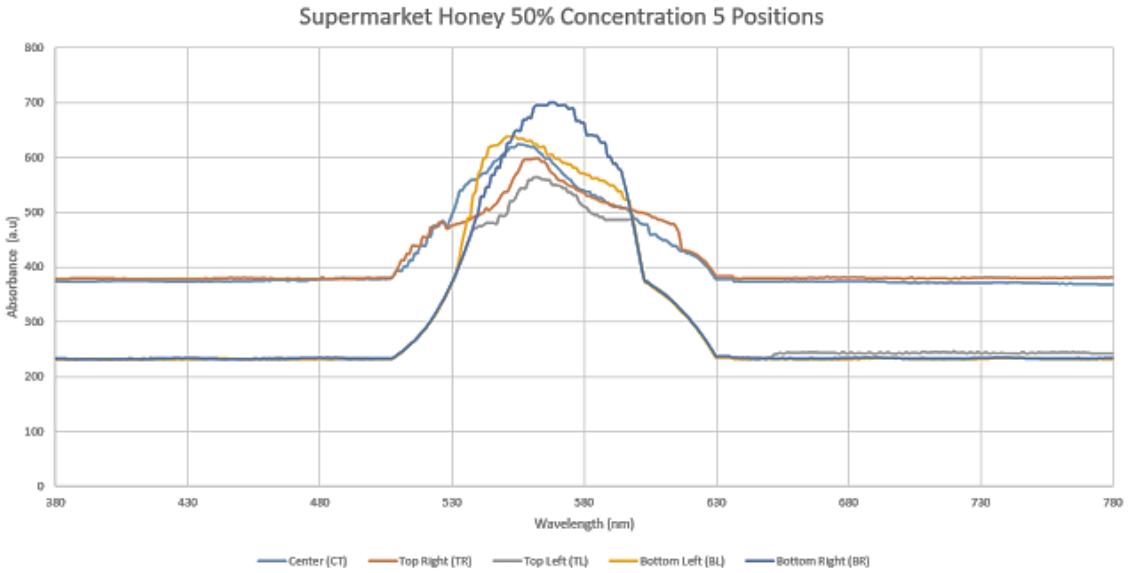

Fig. 6. Graph of absorbance vs. wavelength of supermarket honey with 50% concentration measured at 5 different positions

Figure 7 shows the graph of average absorbance vs. wavelength of supermarket honey with 50% concentration. Note that the sensor in this spectroscopy differs from those in commercial models, so absorbance values may not match those from market spectrometers. The average peak absorbance for supermarket honey 50% concentration is 620a.u at 562nm and surprisingly this is somewhat accurate compared to the actual result from the actual spectroscopy with error margin of ±15nm.

The peak wavelength of supermarket honey measured by Dafni *et al.*, [25] using UV-VIS spectroscopy ranges from 220nm to 550nm. The peak wavelength results from the proposed device are 562nm. This showed that the proposed spectroscopy is reliable to measure supermarket honey as the result is not much different with the actual data taken using actual spectroscopy. This shows that the XY axis really improves the accuracy and sensitivity. However, some noises are recorded where there are three additional lower peaks. These noises are caused by the electromagnetic interference as there is a green light transmitted by the sensor. Overall, this result suggests that the proposed device performs as expected.

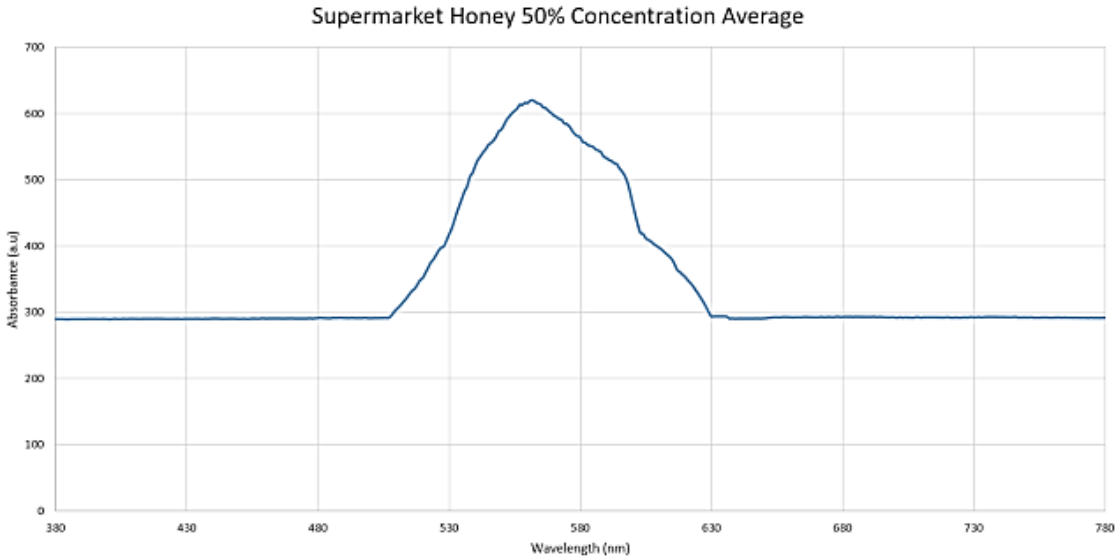

Fig. 7. Graph of average absorbance vs. wavelength of supermarket honey with 50% concentration

4. Conclusions

The development of the proposed non-invasive and portable spectroscopy represents a significant advancement in analytical devices. This innovative technology offered numerous benefits and opportunities across various industries. By eliminating the invasiveness of traditional methods, it preserves the integrity of liquid-based samples, allowing for further analysis and potential reuse, thus minimizing waste and maximizing resource efficiency. The portability of the device enables on-site analysis, fieldwork, and point-of-care applications, revolutionizing sample identification and analysis. Its compact design and ease of use enhanced 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. The accuracy of the device is high and meets expected results, although some noise may still be present as there is an electromagnetic interference as there is a green light transmitted by the sensor.

In summary, the non-invasive and portable spectroscopy is a big step forward in analytical technology. It can analyze liquid samples accurately without being invasive and is easy to use and portable. Using this technology in everyday work can make processes more efficient, cut down on

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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