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Evaluation of the Potential Application of a Portable and Wireless Spectrometer in the Forensic and Medical Field

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Abstract

The application of a wireless portable spectrometer for the quantitative detection of Gamma-hydroxybutyrate (GHB), a commonly abused drug, was explored. Unlike existing portable tests that only detect the presence of GHB, the developed method provides quantitative information. The previously published colorimetric test, involving the formation of the ferric complex of GHB, was modified for spectrometric detection. The absorbance of the purple ferric complex exhibits a linear relationship with the concentration of GHB, showing an average coefficient of determination (r^2) value of 0.7676. The reproducibility of the developed method was evaluated through an inter-day study of the calibration curve. Results indicate that the method for spectrometric detection of GHB has good precision (RSD = 5.94%).The performance of the wireless portable spectrometer for detecting GHB using the developed method was compared with that of a benchtop spectrometer. Results show that the r^2 value for the wireless portable spectrometer and the benchtop spectrometer is 0.8178 and 0.7532, respectively. This suggests that the performance of the portable spectrometer is comparable to that of the benchtop spectrometer. It is demonstrated that the wireless portable spectrometer can perform quantitative analysis for GHB and has potential for onsite application at crime scenes and first response sites.

Introduction

According to the National Institute of Drug Abuse (NIDA), there are 107,471 drug overdoses reported in 2022 in the United States (NIDA, 2024). The most used screening drug tests at the crime scene are simple/rapid drug test kits such as paper-based devices (Da Silva, 2018), detection straws (Bradley, 2011), and swab-based test kits (Callahan, 2017) which mainly rely on color tests. However, these test kits have a false-positive rate of as high as 53.8% due to misinterpreting ambiguous color changes (Park, 2023). Thus, it is essential to develop more selective onsite drug detection methods using portable devices.

Ideally, these portable devices should be capable of performing quantitative analysis onsite, providing crucial information for the treatment of overdose patients. Traditionally, this information is not available until patients are transported to emergency rooms in hospitals and undergo corresponding laboratory tests. Past research has indicated a strong correlation between Emergency Department Length of Stay (EDLOS) and the waiting times for laboratory results, including blood tests, X-rays, and CT scans from diagnostic laboratories (Gardner, 2007; Kocher, 2012). For example, according to the study conducted by Vrijsen et. al (Vrijsen, 2022), shorter turnaround times for laboratory tests are linked to shorter EDLOS. This includes the time taken for blood tests, X-rays, and CT scans. The study also shows that the time to testing (TTT) and the turnaround time (TAT) for these diagnostic tests positively correlate with EDLOS. Essentially, the faster the results are available, the shorter the patient's stay in the emergency department. This relationship is vital because extended EDLOS can lead to overcrowding, which may result in poorer patient outcomes, such as higher rates of mortality and morbidity (Farimani, 2024). Thus, improving the efficiency of diagnostic laboratories can be a crucial approach to decreasing EDLOS and improving overall patient care in emergency departments.

One possible way to increase the efficiency of diagnostic laboratories at hospitals is the ability to collect preliminary quantitative analysis data onsite, before the patients arrive at the hospital. In this way, patients can be treated more efficiently at the hospital. Common portable drug detection devices that can provide quantitative data include sensors and portable mass spectrometry. For example, portable mass spectrometry has been applied to detect drug abuse (Borden, 2022), including fentanyl analogs (Sisco, 2017). Sensors are utilized to detect cocaine (COC), tetrahydrocannabinol (THC), methamphetamine, amphetamine, fentanyl, opioids (morphine, codeine), heroin, and benzodiazepine (alprazolam, chlordiazepoxide, diazepam, oxazepam, and clonazepam) (Ahmed, 2020). However, there has been limited advancement in the onsite quantitative analysis of Gamma-hydroxybutyrate (GHB).

GHB is known for its abuse potential and acts as a powerful central nervous system depressant. It is frequently encountered in forensic investigations involving both living and deceased individuals. Small amounts of GHB (0.5-1.0 mg/L) are naturally produced in various tissues (Crookes, 2004; Elian, 2002) including the brain, where it serves as both a precursor and a metabolite of the primary inhibitory neurotransmitter γ-aminobutyric acid (GABA) (Wong, 2004; Tunnicliff, 1997). The sodium salt form of GHB, marketed as Xyrem (Pardi, 2006; Robinson, 2007; Carter,2009) is approved in some countries for treating cataplexy associated with narcolepsy (Dauvilliers, 2007).

GHB is a commonly abused drug by teens and young adults at all-night parties and "raves" (Maxwell, 2005; Ghosh, 2019). It is classified as a Schedule I-controlled substance and is typically available as a white powder or a clear liquid. It is often misused for its euphoric and sedative properties (Drug Enforcement Administration, 2022). When combined with alcohol, its effects can be amplified, leading to respiratory depression and coma. Street names for GHB include Easy Lay, G, Georgia Home Boy, GHB, Goop, Grievous Bodily Harm, Liquid Ecstasy, Liquid X, and Scoop (Department of Justice, 2020).

The initial effects typically manifest within an hour and may include rapid heart rate, enlarged pupils, high blood pressure, elevated body temperature (Bakheit, 1990; Friedman, 1971; Mercieca, 1984) and goosebumps. The risk of death from GHB abuse is significant due to the small safety margin between a recreational dose and a lethal dose, which ranges from just 5:1 to 8:1. Consequently, accidental overdoses from recreational use of GHB are relatively common, as indicated by frequent hospital emergency department admissions and forensic medical investigations into drug-related deaths (Caldicott, 2004; Knudsen, 2008; Knudsen, 2010; Gable, 2004; Schulz, 2012). According to the study by Park et. al. (Park, 2023), it is essential to address the limitations of current GHB detection kits, enhance their detection capabilities, and develop more reliable kits. The purpose of this study is to evaluate the potential application of a portable, wireless spectrometer for onsite quantitative detection of GHB. Initially, the functionality of the wireless spectrometer is assessed using a purple commercial vegetable dye and compared with a benchtop spectrometer. Subsequently, the colorimetric test published in a previous study for GHB detection (Alston, 2002) is modified and adapted for spectrometry measurement. Quantitative measurements are then conducted using both the benchtop and wireless spectrometers with standard GHB solutions. The results are compared and evaluated.

Experimental and Results

Material and Instrumentation

The wireless portable spectrometer (Model: Pasco 2600A) was from Pasco Scientific (Roseville, CA, U.S.A.) Data was collected wirelessly on Samsung Galaxy Tab with the SPARKvue app. The benchtop UV/Vis spectrometer (Model: Evolution 300) was from Thermo Fisher (Waltham, MA). Vegetable dye (FD&C Wool Violet 5BN) was from ScholAR Chemistry (manufactured by Aldon Corp, Avon, NY, U.S.A.). The sodium salt of Gamma-hydroxybutyric acid (GHB) was obtained from Sigma Aldrich (St. Louis, MO). Hydroxylamine hydrochloride ($NH_3OH.Cl$), ferric chloride, sulfuric acid, sodium hydroxide, and pH paper were obtained from Fisher Scientific Inc. (Tustin, CA). All reagents were analytical grade, and all solvents were HPLC grade.

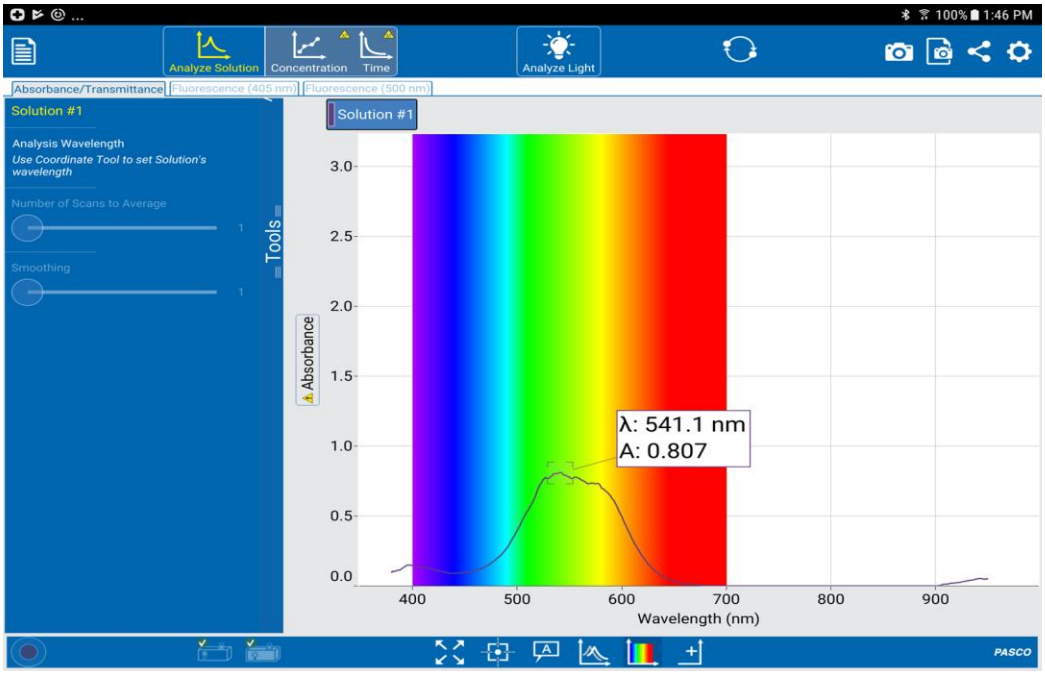
Part I Evaluation of a Wireless Portable Spectrometer Using a Purple Commercial Vegetable Dye

Determination of the Connectivity Range of the Wireless Portable Spectrometer

The maximum connectivity range of the wireless portable spectrometer was determined by gradually moving the Samsung tablet away from the spectrometer until the signal was lost. The connectivity range was found to be 60 feet.

Determination of Maximum Absorbance Wavelength (λ_{max})

A primary stock solution was prepared by pipetting 1 mL of the purple commercial vegetable dye into a 10-mL volumetric flask and diluting to mark with distilled water. A working stock solution was prepared from the primary stock solution with a 1:80 dilution and was assigned an arbitrary concentration of 1.00 unit (a.u). A standard solution with an arbitrary concentration of 0.75 a.u. was prepared from the working stock solution. The maximum absorbance wavelength (λ_{max}) was determined by filling a cuvette with a 1.0 cm pathlength with the standard solution (0.75 a.u) and inserting it into the spectrometer. The spectrum was collected on a Samsung Galaxy Tab using the SPARKvue app. Figure 1 shows the collected spectrum. The wavelength with the maximum absorbance (λ_{max}) was found to be 541.1nm.



Solution #1

Analysis Wavelength

Use Coordinate Tool to set Solution's wavelength

Number of Scans to Average 1

Smoothing 1

Figure 1. Spectrum for Purple Commercial Vegetable Dye Collected at the Portable Wireless Spectrometer

Regression Analysis

Standard solutions with arbitrary concentrations of 0.75, 0.25, 0.125, and 0.0625 a.u. were prepared from the working stock solution with an arbitrary concentration of 1.00 as described in the previous section. A calibration curve was generated by taking absorbance measurements for each standard solution at λmax (541.1 nm) using a cuvette with a 1-cm pathlength (Figure 2).

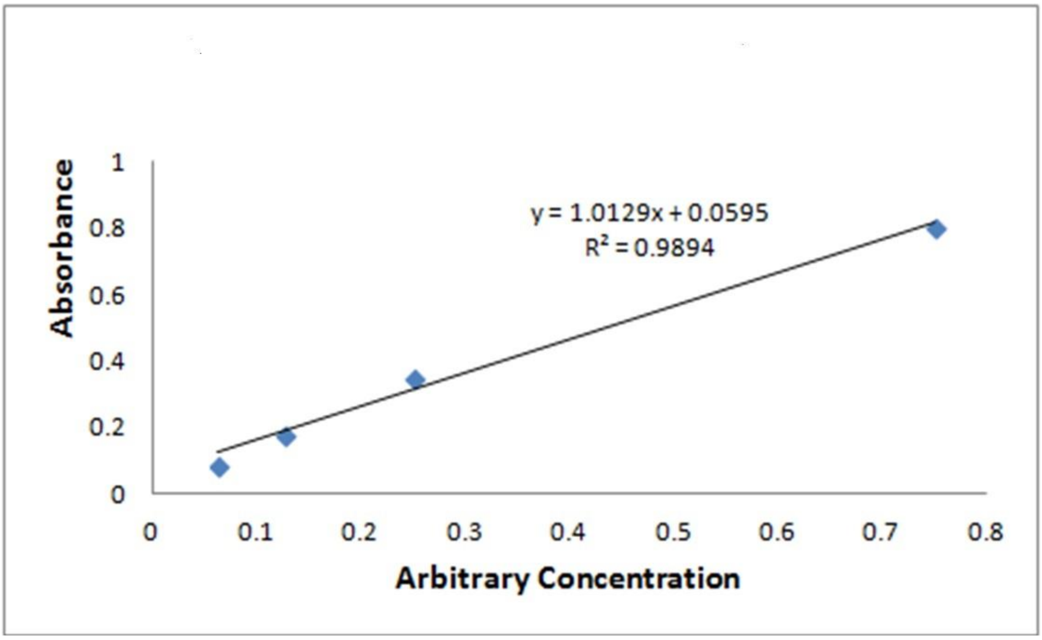


Figure **2**. Calibration Curve of the Purple Commercial Vegetable Dye Using a Cuvette with a 1.0-cm Pathlength at the Portable Spectrometer.

Comparison Studies on Pathlength

In the medical and forensic fields, it is desirable to perform analyses with minimal sample sizes. Therefore, a calibration curve was generated by measuring absorbance using a cuvette with a 0.2 cm pathlength (Figure 3).

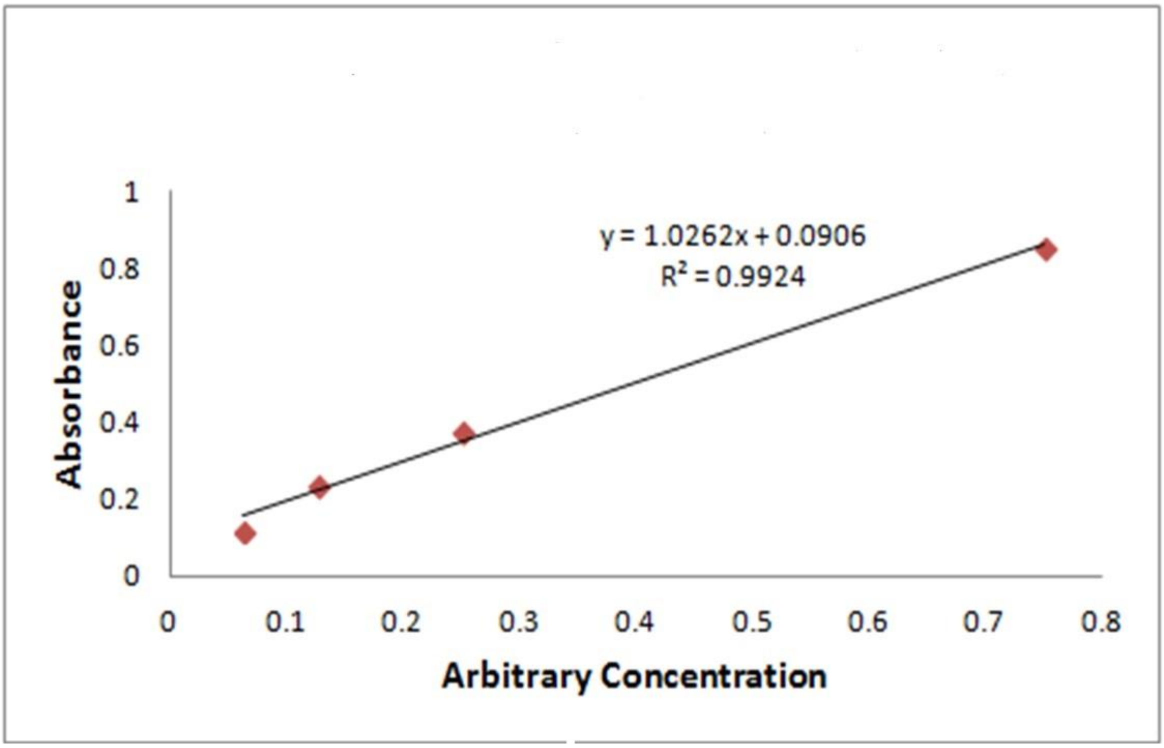


Figure 3. Calibration Curve of the Purple Commercial Vegetable Dye Using a Cuvette with a 0.2-cm Pathlength at the Portable Spectrometer.

Estimation of Beam Height in the Portable Wireless Spectrometer

The beam height of the radiation source in the portable wireless spectrometer was determined by comparing absorbance measurements at different sample heights in the cuvette. Measurements were taken at 541.1 nm using a purple commercial vegetable dye standard solution with a concentration of 0.25 a.u. Absorbance was measured with the cuvette (1.0 cm pathlength) filled to its full volume capacity and half of its volume. The results are presented in Table 1.

Table 1. Absorbance Measurement of Purple Dye Standard Solution (0.25 a.u.)

Height of solution in the Cuvette	**The volume of the solution in the Cuvette**	**Absorbance at 541.1 nm**
4.420 cm	4.12 mL	0.616
2.246 cm	2.06 mL	0.616

Comparison Study with a Bench Top UV/Vis Spectrometer

A primary stock solution was prepared by pipetting 5 ml of the purple commercial vegetable dye into a 10-mL volumetric flask and diluting to mark with distilled water. A working stock solution was prepared from the primary stock solution with a 1:50 dilution and was assigned an arbitrary concentration of 2.00 units (a.u).Standard solutions with arbitrary concentrations of 1.6, 1.2, 1.0, 0.8, 0.5, and 0.25 a.u. were prepared from the working stock solution. Calibration curves were prepared by measuring the absorbance of these standard solutions at 542 nm using a cuvette with a 1.0- cm pathlength on both the portable and benchtop spectrometers (Figure 4).

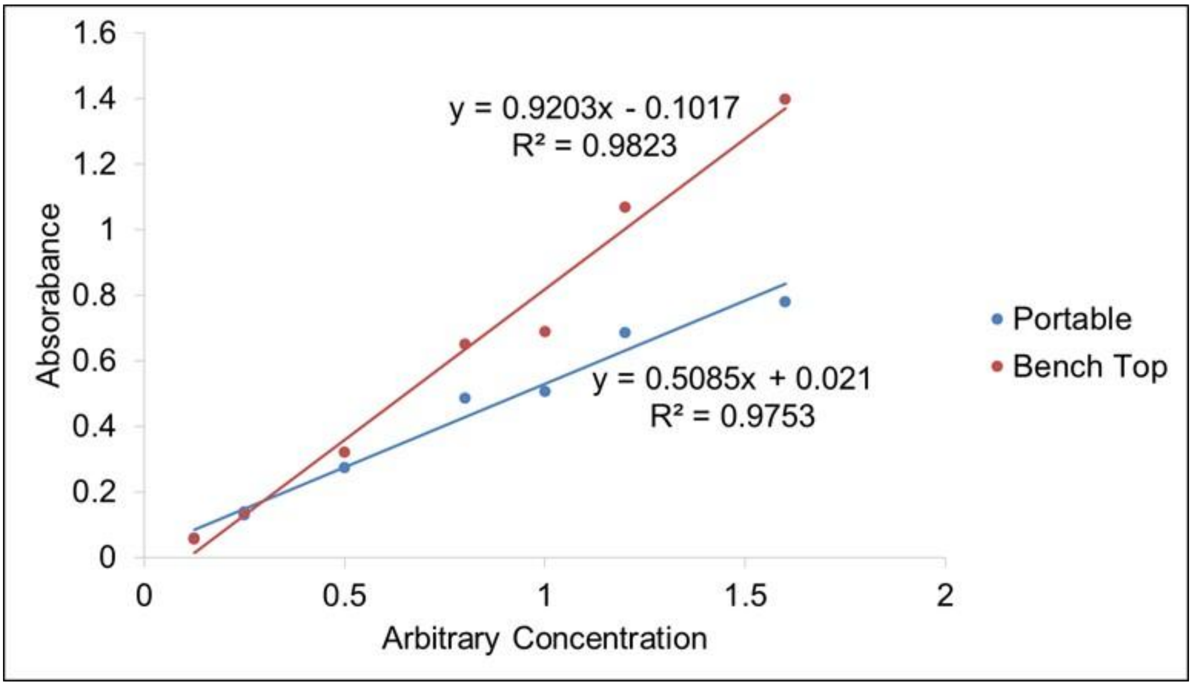


Figure 4. Calibration Curves for Purple Commercial Vegetable Dye Utilizing (a) a Portable Spectrometer, and (b) a Benchtop Spectrometer

Part II Spectrometric Detection of *Gamma-Hydroxybutyrate* (GHB)

Adaptation of Colorimetric Test for Gamma-Hydroxybutyrate (GHB) in Spectrometry Measurement

The concentrations and volumes of sodium hydroxide and sulfuric acid in the previously published colorimetric test for GHB (Alston, 2002) have been adjusted to perform the reaction within a cuvette (volume = 4 mL, pathlength = 1 cm) for immediate spectrometry measurement once the purple color develops. The adjusted procedures is as follow: (1) 0.3 mL of the GHB solution is added to the cuvette, (2) followed by 0.5 mL of 3.0 M H_2SO_4, (3) 1 mL of 0.5 M NH_3OHCl,(4) the pH is adjusted to 10 by adding 1.26 mL of 3M NaOH, (5) 0.4 mL of 3M H_2SO_4 is added to adjust the pH to 2, (5) 0.2 mL of 0.7 M $FeCl_3$ is added to develop the instant purple color.

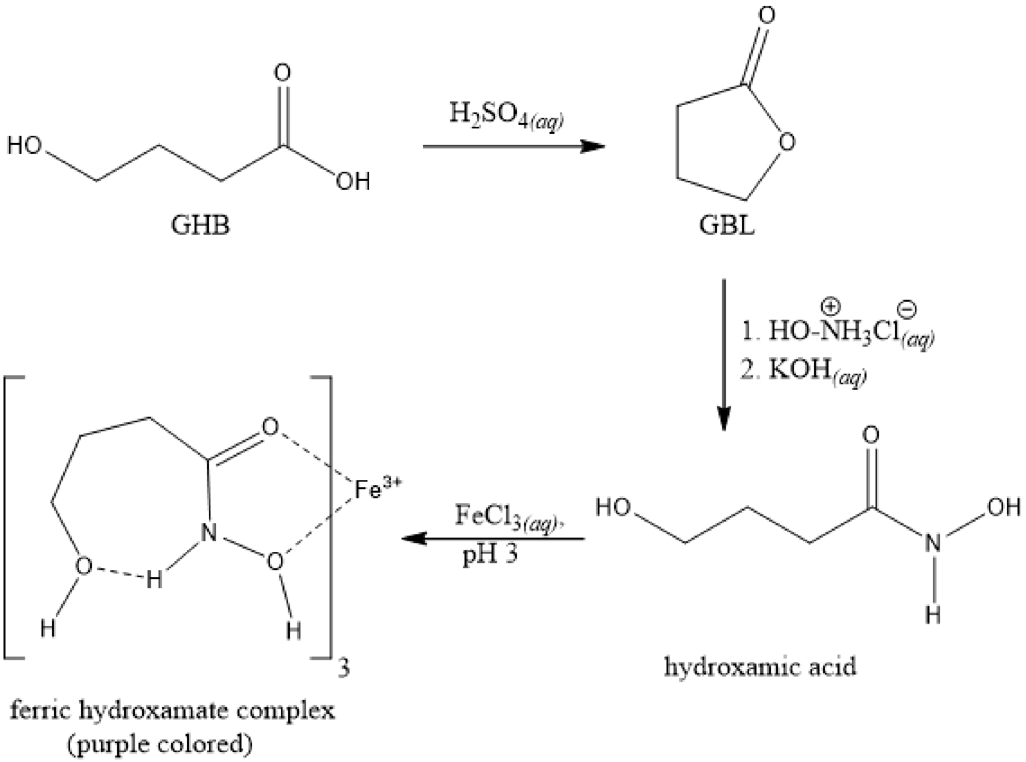


Figure 5**.** Ferric Hydroxamate GHB Colorimetric Assay Reaction Sequence (Alston, 2002).

Determination of Maximum Absorbance Wavelength (λ_{max}) of the Purple Complex

A 1.0 mg/mL standard solution of GHB was used. The purple color was developed using the procedure described above. The absorbance spectrum of the resulting purple colored complex was collected by scanning from 400 to 800 nm. The wavelength with the maximum absorbance (λ_{max}) was found to be 500 nm.

Study on the Effect of GHB on The Absorbance of the Developed Purple Complex

A 10.0 mg/mL stock solution of GHB was prepared by accurately weighing the sodium salt of Gamma-hydroxybutyric acid (GHB) at the balance and dissolved it in distilled water. Five GHB standard solutions with concentration of 1.0, 2.0, 3.0, 4.0, and 5.0 mg/mL were prepared from the 10.0 mg/mL stock solution. The purple color was developed for each standard solution as described above and the absorbance of the developed purple color was measured at 500 nm using the portable wireless spectrometer. A calibration curve was prepared by plotting absorbance versus concentration of the GHB.

Inter-Day Study

The reproducibility of the method was evaluated by repeating the color development for each standard solution and measuring the corresponding absorbance on three different days. A total of three runs were performed. The r^2 value for each run and the relative standard deviation (RSD) are shown in Table 2.

Table 2. Summary of the Coefficient of Determination (r^2) Value Of Calibration Curves

Run	r^2 value of the calibration curve	
1	0.7317	
2	0.8178	Average = 0.7676
3	0.7533	RSD = 5.94 %

Comparison Study with a Benchtop UV/Vis Spectrometer

Calibration curves were prepared as described above. The absorbance of the developed purple color for each standard solution was measured at 500 nm using both the benchtop UV/Vis spectrometer and the portable spectrometer. The calibration curves are shown in Figure 6.

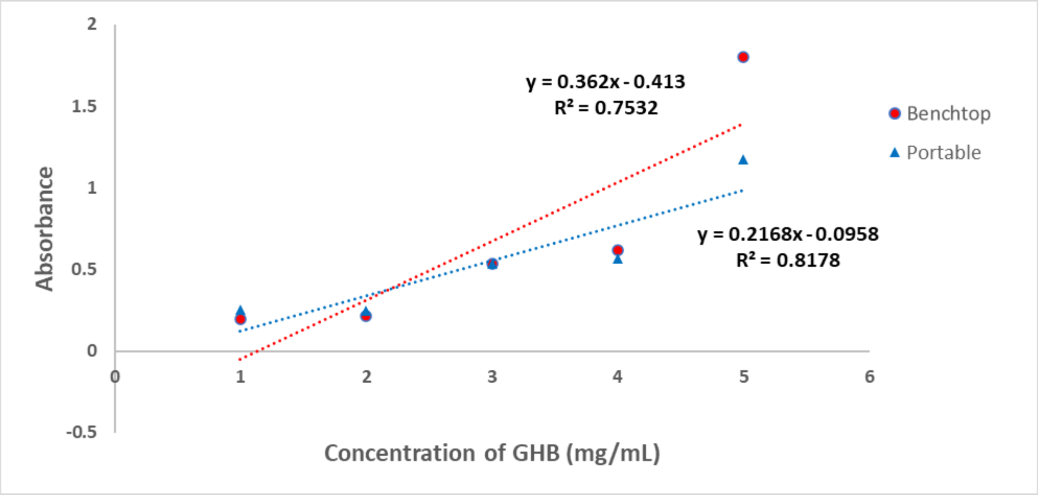


Figure 6. Calibration Curve of GHB Utilizing (a) a Benchtop Spectrometer and (b) a Portable Spectrometer

Discussion and Conclusions

Part I. Evaluation of Wireless Portable Spectrometer with Commercial Dye

The wireless portable spectrometer has a connectivity range of 60 feet. The maximum absorbance wavelength for the purple dye is 541.1 nm. Calibration curves of purple dye with 1.0 cm and 0.2 cm pathlengths show good coefficient of determination (r^2) values of 0.9894 and 0.9924, respectively. It is concluded that when sample size is limited, measurements can be made with a cuvette with a 0.2 cm pathlength. The absorbance signals for fully filled and half-filled cuvettes are approximately the same, indicating that the beam height is about half the height of the cuvette (22.46 mm). The r^2 value obtained from the wireless portable spectrometer (0.9753) is comparable to that of the benchtop UV/Vis spectrometer (0.9823).

Part II. Spectrometric Detection of GHB

The previously published color test that involves the formation of the ferric complex of GHB has been successfully modified for spectrometric detection. The absorbance of the purple ferric complex formed inside the cuvette was measured immediately after the color was developed. The absorbance of the purple ferric complex shows a linear relationship with the concentration of GHB, indicating a substantial dependence between the two. The reproducibility of the developed methods was evaluated through an inter-day study of the calibration curve. The study demonstrated an average r^2 value of 0.7676 and a relative standard deviation (RSD) of 5.94%, indicating good precision for the spectrometric detection of GHB. Furthermore, the performance of the wireless portable spectrometer for the detection of GHB using the developed method was compared with that of the benchtop spectrometer. Results show that the r^2 value for the wireless portable spectrometer and benchtop spectrometer is 0.8178 and 0.7532 respectively. This suggests that the performance of the wireless portable spectrometer is comparable to that of the benchtop UV/Vis spectrometer. It also indicates that the wireless portable spectrometer can produce high-quality, dependable data despite its small and mobile design.

Overall Conclusions

A new application of the wireless portable spectrometer for quantitative detection of gamma-hydroxybutyrate (GHB), a frequently abused substance, has been developed. Detecting GHB is crucial in both medical and forensic settings due to its potential for abuse and its role in various criminal activities, such as drug-facilitated sexual assault. The wireless portable spectrometer’s capability to provide precise and quantitative GHB analysis, along with its potential for onsite application, could be highly beneficial for clinical and forensic purposes. In medical settings, it might quickly evaluate patient samples, aiding in the prompt diagnosis and treatment of GHB intoxication. In forensic investigations, it could enable immediate evidence analysis at crime scenes, which is crucial for the timely collection and preservation of data. One of the key advantages of this method is its potential to deliver ‘just in time’ information. This means that data could be obtained and analyzed efficiently, greatly accelerating the decision-making process. For healthcare providers, this might result in faster patient care and improved outcomes. For forensic investigators, it could enhance the efficiency and accuracy of crime scene investigations, potentially leading to quicker resolutions and stronger legal cases. Incorporating this wireless portable spectrometer into regular practice might significantly boost efficiency in both clinical and forensic fields. The potential ability to perform onsite analysis could reduce the need for sample transportation and the associated delays. This might not only save time but also reduce the risk of sample degradation or contamination, ensuring more reliable results.

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