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# Creation of a Portable, 3D-Printable, iPhone-Compatible Spectrophotometer

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# Creation of a Portable, 3D-Printable, iPhone-Compatible Spectrophotometer

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*Spectroscopy, Visible Light, Technology*

## Abstract

Spectroscopy is a widely used chemical and medical analysis tool. While spectrophotometers are commonly found in many universities and laboratories, they are not available to all high schools or laboratories in developing countries. The objective of this project was to design a high-quality, 3D-printable, iPhone-compatible spectrophotometer that uses a cell phone camera and interface to collect data. The created 3D-print file will be available to anyone with access to a 3D printer which are increasingly found in many laboratories and schools across the country. A low cost pre-printed kit will also be made for those without access to a 3D printer compared to any other commercial system. This spectrophotometer design will expand the number of people that have the capacity and ability to utilize this type instrumentation. For educational purposes, there are several protocols that can be utilized with the cell phone spectrophotometer to help students greater understand the principles of color, wavelength, light, absorbance, transmittance, and the science of spectroscopy. The cell phone spectrophotometer was compared to three widely used commercial spectrophotometers for concentration versus absorbance for a red solution. The absorptivity values are 0.687±0.002, 0.638±0.011, 0.629±0.004, and 0.436±0.023 for the Cary Spectrophotometer, Nanodrop 2000, Spectrometer 21, and SpecPhone respectively.

## Introduction

Spectroscopy is an essential tool chemists use to analyze and quantify molecules and atoms. The principles of color, wavelength, visible light, and transmission are all an integral part of spectroscopy. In basic chemical research, the reaction of a substrate to produce a colored solution is often used to quantify reactant/product concentrations and reaction kinetics. In biochemistry research, spectroscopy is often used in enzyme assays to determine concentration or binding affinity.[1] In a clinical setting, spectrophotometry is an essential tool to analyze and report crucial health information, like cholesterol levels.[2] Inevitably, the concepts behind spectrophotometry are important for a wide range of STEM and health professions.

At the collegiate level, UV-Visible light spectroscopy is taught with the basic principles of Beer-Lambert's Law. Conceptually, teaching these principles can be improved with laboratory exercises to reinforce the concepts and help the students develop an experiential knowledge of the subject. Unfortunately before college, students are not exposed to the methodologies and experimentations associated with spectrophotometers due to the limitation of resources and funding. UV-Visible light spectrophotometry is not typically taught at the high school level, but could be with improved and cheaper instrumentation. Greater access to the tools of spectrophotometry could greatly improve comprehension so that the concepts do not become a stumbling block in college. An educational movement has been emphasizing experimental-facts-first model, instead of the traditional atoms-first model.[3] This educational technique more similarly reflects the scientific method and allows students to explore the field of chemistry in an experimental environment, much like the professional world.[4] Spectroscopy allows students to connect with scientific theories in an experimental and macroscopic manor.

Resource and funding are just two challenges faced by educators to integrate scientific techniques and machinery into primary/high school education. Research grade instruments are very expensive. Educational versions are also expensive and have many educational drawbacks. In UV-Visible light spectrophotometers, there is an element of a 'black-box' phenomena. The students place a sample in the instrument and the instrument gives an absorbance or transmittance value. There is no current technical tool to visibly see the spectra that the colored sample is giving off. Many manufacturers have already attempted to emulate spectrophotometers that are inexpensive and use visible light.[5] Some instruments have the ability to see the spectra, yet not analyze and quantify the results.[6] Others need a connection to a computer while in use.[6] Combining the elements of a visual spectra with the ability to analyze and quantify data at a low cost is the optimal solution.

A spectrophotometer is created using 3D-print technology and a universal engineering programming (SolidWorks). SolidWorks is a CAD (computer-aided design) software that is utilized by many universities and scientists. A cellular phone (iPhone 5) is used as the interface to collect the spectral images. An iPhone is chosen based on popularity and occurrence across the world. The spectrophotometer file is created on SolidWorks, converted to a 3D-print file, and printed on the Cube 2 3D printer.

## Design

A first prototype was designed based on visible light and spectrophotometer properties. It was known that a mirror, diffraction grating, slit, white light source, and iPhone would be utilized in the design. A known limitation was the size of the 3D printer base. The end product would need to be no larger than a 5 inch cube so that it could be printed on any consumer-grade 3D printer. There are certain elements of every spectrophotometer that needed to be incorporated. The light used to illuminate a sample needs a path that includes a slit, the sample, and a detector to collect the spectra in that order. A slit insert was created just past the point of light entry in the spectrophotometer. A slit is not only needed to create a uniform path of light through a sample to the detector, but also to increase the resolution of the dispersed wavelengths of the visible spectrum. In this design, the slit can be removed and changed to fit many variables. Based on calculations, the ideal slit width for this design is 0.1 cm. Inside the spectrophotometer, there is a mirror to reflect the light at a 45 degree angle to the detector, the iPhone camera. The iPhone is resting at a 45 degree angle on the spectrophotometer and therefore the reflected light creates a 90 degree angle. A grating of 1000 lines/mm is mounted at the front of the spectrophotometer just under the camera interface.  The grating is needed to disperse the colors of light from white light to create a spectra. Based on these properties, Figure 1 shows the first version of the spectrophotometer in a SolidWorks file. To ensure consistency and ease of use, a mount was created for the iPhone. The assembly of this mount with the spectrophotometer is shown is Figure 3. The supplies needed to finish the spectrophotometer product and source are listed in table 1.

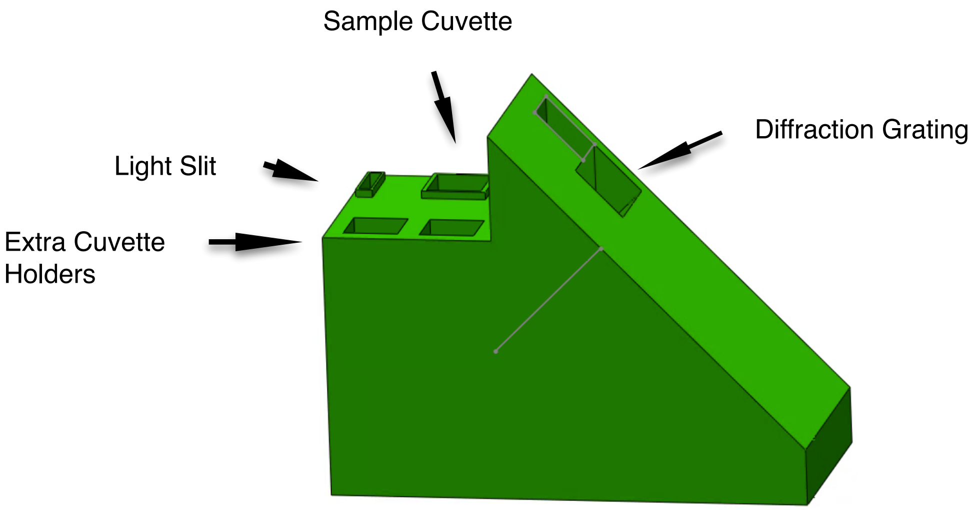


Figure 1: First Version of the Spectrophotometer. The required elements are incorporated without a case for the iPhone to be fixed on the spectrophotometer. The drawing and image was created using SolidWorks version 64, 2014.

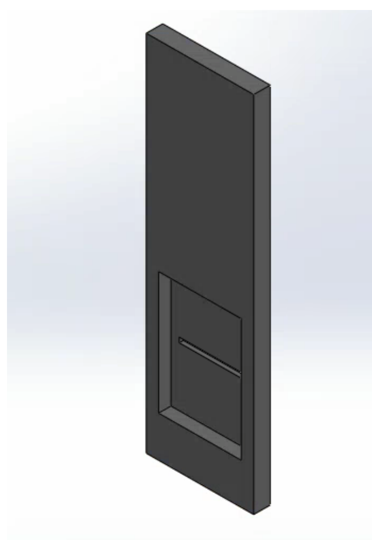

Figure 2: Removable Slit. This slit allows the white light source to be directed in such a way that only passes through the sample of interest. The drawing and image was created using SolidWorks version 64, 2014.

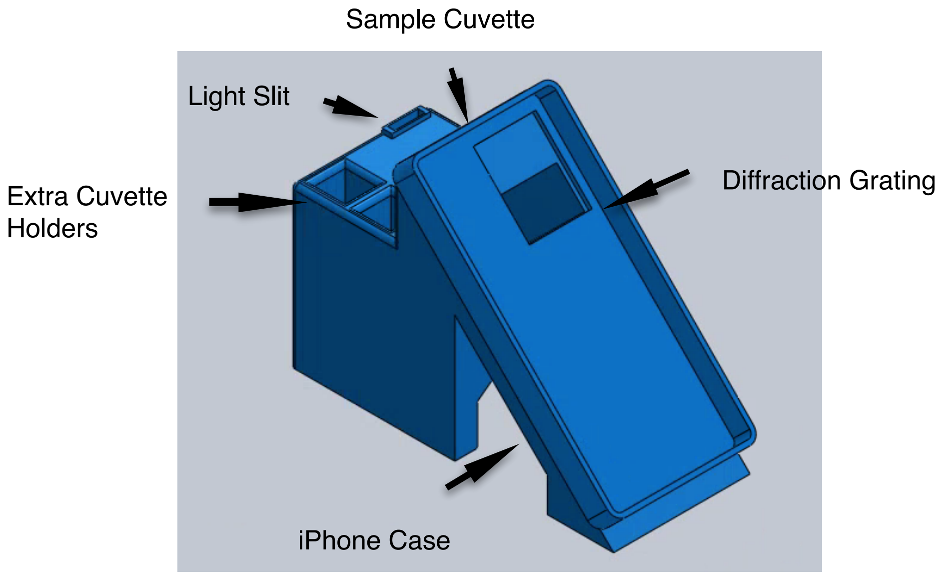


Figure 3: Assembly of the spectrophotometer. There are positions for an adjustable light slit, cuvette sample holder, two extra cuvette holders, a diffraction grating, and iPhone case aperture. The drawing and image was created using SolidWorks version 64, 2014.

| Material | Source | Price |
|---|---|---|
| Diffraction Grating | amazon.com | $14.95 (package of 25) |
| Square Mirror | Art Supply Store/ Oriental Trading Company | $7.25 (package of 400) |
| White Light Source | Any Department Store | $5 and up |
| Cuvettes | Vernier Products | $15 (package of 100) |
| iPhone | Personal Property or Electronic Store | $0-$150 |

Table 1: Extra supplies cost and source. The designed cell phone spectrophotometer is reasonable for many middle/high school and collegiate level funding.

## Assembly

After printing the body of the spectrophotometer, the assembly is quite simple. First, the mirror is to be placed inside the spectrophotometer from the front opening. It is suggested that a piece of double-sided tape is utilized to keep in place. Then a small square of the diffraction grating should be cut (approximately 1*1 square inch) and adhered to the top front of the spectrophotometer. The white light source should be placed at the back of the spectrophotometer at a fixed position between each data sample collection. The iPhone is then to be placed in the mount and the camera application opened for collection. The removable slit should be placed in it's location directly behind the cuvette of interest. As needed, add the cuvette with the sample of interest into the cuvette slot adjacent to the slit and take pictures of the spectra on the cellular phone.

## Protocols

For the cell phone spectrophotometer, there are two academic levels in which this scientific instrument can be utilized. The first occurs at an upper elementary/middle school range. The students would use the spectrophotometer to visually explore the properties of color and wavelength. The students can make various colored solutions with either Kool-aid or food dye. One at a time, the colored solutions would be placed in a plastic cuvette and then into the spectrophotometer. The spectra is visible on the cell phone screen and can easily be compared to the full spectra by lifting the cuvette out of the holder. The visual stimulus gained form this experiment can engage students in the ideas between visible light absorbance and transmittance. The protocol answers questions such as "What color disappears (is absorbed) when another is placed in the spectrophotometer?" and "How do each of the colors of the spectra relate to a wavelength value?".

The second protocol occurs at a high school/collegiate range. The students would use the spectrophotometer to measure spectra at different solution concentrations to determine absorbance at a particular wavelength.[7] This protocol also allows for students to learn how to perform serial dilutions. Students would begin with one colored Kool-aid or food dye. A stock solution would be made to begin the serial dilutions. Each different solution in the dilution would be placed in a plastic cuvette and a spectral image would be taken. These images can be run through a program called imagej to collect light transmittance per pixel space. From these data, absorbance can be calculated using Beer's Law. The spectral peak can be chosen (or a particular wavelength) to plot absorbance versus concentration. This creates a graph and visual conformation of a linear correlation between the solution concentration and absorbance. The protocol answers questions such as "Does absorbance increase or decrease in relation to solution concentration?" and "How do the spectral images appear as solution concentration changes?".

## Results

The protocol set up for high school/collegiate level students was used to evaluate the efficiency of the cell phone spectrophotometer. Cherry Kool-aid was used as a red solution concentration determinant. 0.4134g was dissolved in 100 mL DI water. From this stock solution, six serial dilutions were made. The same colored solutions were evaluated by a Nanodrop 2000, CarySpec, Spec21, and the cell phone spectrophotometer. Absorbance versus concentration were plotted according to the Nanodrop, CarySpec, and Spec 21. The absorbance was determined for the cell phone spectrophotometer by putting the images through a program called imagej. Imagej first takes the seven different images and creates a stack. This stack places the spectra in sequential order (from least to greatest solution concentration) and directly on top of one another. Imagej then plots a profile of the transmittance versus pixel position. From here, simple excel data analysis calculates transmittance per pixel position to absorbance per pixel position. The peak absorbance for each solution concentration is found and plotted against concentration. The results for each spectrophotometer appear below in chart 1 corresponding with table 2.

| | | Absorbance at 496 nm | | | |
|---|---|---|---|---|---|
| | **Concentration (mg/mL)** | **Nanodrop 2000** | **Spectrometer 21** | **CarySpec** | **SpecPhone** |
| **Solution G** | 0.06451563 | 0.03 | 0.025 | 0.037 | -0.0175 |
| **Solution F** | 0.12903125 | 0.04 | 0.07 | 0.082 | -0.0139 |
| **Solution E** | 0.2580625 | 0.13 | 0.16 | 0.175 | 0.0591 |
| **Solution D** | 0.516125 | 0.32 | 0.32 | 0.356 | 0.1663 |
| **Solution C** | 1.03225 | 0.65 | 0.65 | 0.710 | 0.4928 |
| **Solution B** | 2.0645 | 1.33 | 1.30 | 1.419 | 0.9057 |

Table 2: Comparison of Commercial Spectrophotometers and the Cell Phone Spectrophotometer for an Absorbance at 496 nm versus Concentration of Cherry Kool-aid Solutions

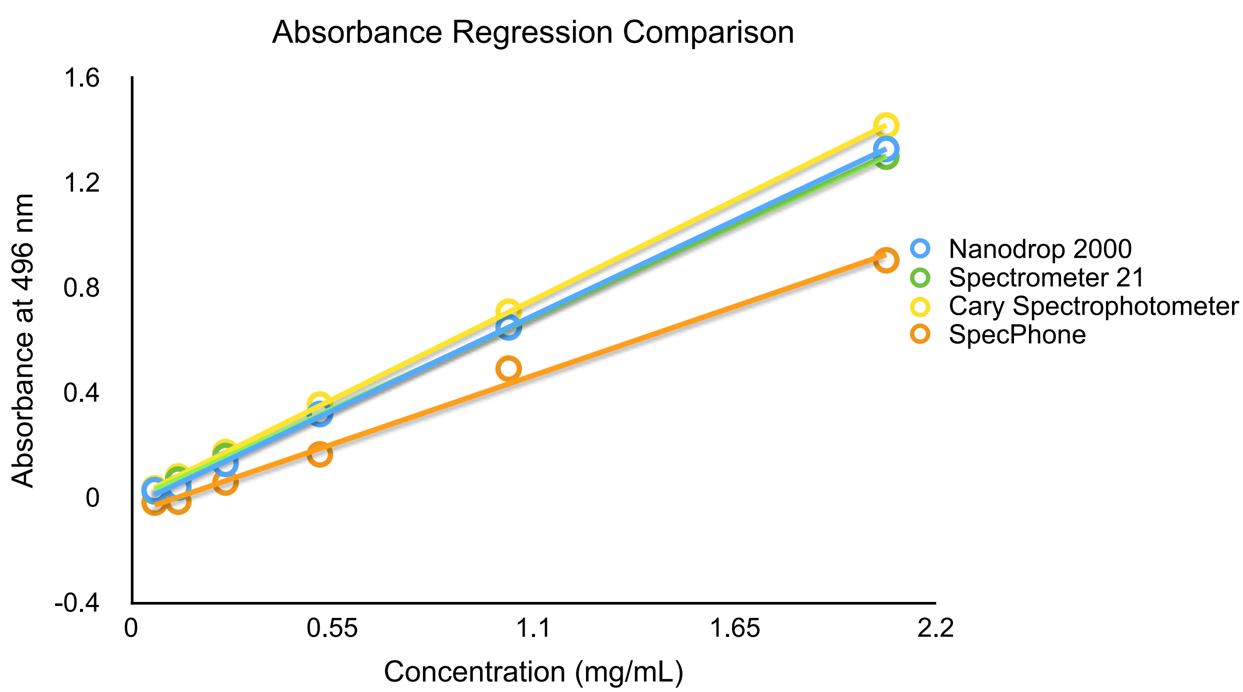


Chart 1: Linear Regressions of Commercial Spectrophotometers and the Cell Phone Spectrophotometer for an Absorbance at 496 nm versus Concentration of Cherry Kool-aid Solutions

A regression analysis was also done on the three commercial spectrophotometer devises and the cell phone spectrophotometer. The results for each spectrophotometer appear below in chart 2 corresponding with table 3.

| | Absorptivity | Std Error | $R^2$ |
|---|---|---|---|
| **CarySpec** | 0.687 | 0.002 | 0.999 |
| **Nanodrop** | 0.638 | 0.011 | 0.998 |
| **Spec 21** | 0.629 | 0.004 | 0.999 |
| **SpecPhone** | 0.436 | 0.023 | 0.986 |

Table 3: Comparison of Absorptivity with Corresponding Standard Errors

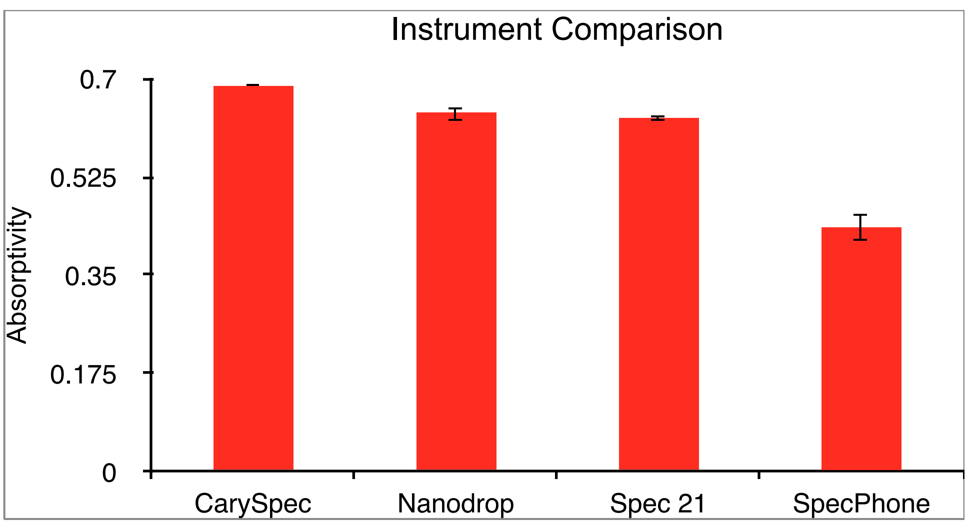


Chart 2: Comparison of Absorptivity with Corresponding Standard Errors

## Discussion

Based on the data collected, the cell phone spectrophotometer $R^2$ value is quite close to the commercial instruments. Although, when absorptivity is calculated (see chart 2), there is a significant difference between the commercial instruments and the cell phone spectrophotometer. The difference is likely due to some combination of the light source and the cell phone camera. In cell phone cameras, there are automated correction factors to the dynamic range that may attenuate the linear response of the ccd pixels to the light intensity. In commercial instruments, the detectors are designed to the light source to be flat across the visible spectrum and to extend above and below the limits of the cell phone camera. This discrepancy may be due to the type of light source used to illuminate the sample. For experiments described like those in the protocols, the difference in absorptivity consistency between the commercial instruments and the cell phone spectrophotometer isn't a problem. Once calibrated, the absorptivity value is valid for the instrument and can be used to determine unknown concentrations in the range we tested. The high school student experiment is used to teach the ideas of spectroscopy and serial dilutions. The evaluation of data is used to understand the importance of serial dilutions and to evaluate concentration versus absorbance. The cell phone spectrophotometer reads and evaluates absorbance quite well.

## Future

The future for this cell phone spectrophotometer is very promising. During a student outreach program called 'King and Friends Science Olympiad', the cell phone spectrometer was used to teach the middle school protocol to 5th and 6th graders. The response was very well taken. The students were able to see the difference in spectra visually between water and a colored solution. The ideas of absorbance and transmittance of light were understood by the students. By the end of the sessions, the students were able to predict which colors would be absorbed/ transmitted when presented with a colored solution of their own. For high school education and clinical settings, a cell phone application development would be ideal. A cell phone application measuring intensity of light per pixel space as soon as an image is taken would eliminate the need for the computer program imagej. Students or clinical evaluators would take the intensity of light per pixel space data directly from the cell phone onto a computer to evaluate via excel. Also for a clinical setting, the light source would need to be narrowed to ensure consistent absorptivity and $R^2$ values compared to commercial systems. In terms of education, this cell phone spectrophotometer could bring a difficult scientific principle to light in younger students. Exposure to scientific principles and interest in scientific experimentation could expand greatly.

The cell phone spectrophotometer is currently going through the patent approval process. From this patent, the CAD/SolidWorks file will be available to the public via the webpage of Dr. Adam W. Smith. This webpage will be the portal between the cell phone spectrophotometer and educators world wide. Anyone with access to a 3D printer, which are increasingly found in many libraries and laboratories, can download the CAD/SolidWorks file for printing. In conjunction with the cell phone spectrophotometer, the protocols and material list will be provided for educators to follow and implement in the classroom. Ideally, a program or press release will be started to raise awareness and interest in the cell phone spectrophotometer. From interest and funds, the printed cell phone spectrophotometer and materials will be available to purchase as a unit.

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## Appendix 1: Safety Considerations

Food Dye Storage: Do not store below 0 degrees C or above 50 degrees C. Store in a cool, dry location. Keep containers tightly closed at all times when not in use. Store in clearly labelled containers.

Food Dye Handling: Avoid skin and eye contact by wearing gloves and goggles. Always wash hands after use. Do not eat, smoke or drink this product.

Kool-aid Storage: Store in a cool, dry location. Keep packages tightly closed at all times when not in use. Store in clearly labelled containers.

Kool-aid Handling: Avoid eye contact by wearing goggles. Gloves may be worn to avoid coloration, but is not hazardous to skin. Always wash hands after use. Do not inhale this product.

Spectrophotometer Handling: There are no optical hazards. Separate samples of interest from white light source and cellular phone to avoid any electrical safety hazards.

Cube 2 3D Printer Handling: Avoid contact with the print head during operation. The print head is extremely hot and can cause burns. If necessary, use an X-acto knife to remove any extra plastic. During removal of the finished printed material, carefully use an X-acto knife or razor blade to clean the print platform. Always wash hands with soap after using the 3D print glue. The glue degrades with soap. Store glue in a cool, dry location.