DETECTION OF PHYSIOLOGICALLY RELEVANT ALCOHOL CONCENTRATIONS USING RAMAN SPECTROSCOPY

A Senior Honors Thesis

by

JOSHUA L. MCKAY

Submitted to the Office of Honors Programs
& Academic Scholarships
Texas A&M University
In partial fulfillment of the requirements of the

UNIVERSITY UNDERGRADUATE
RESEARCH FELLOWS

April 2006

Major: Biomedical Engineering

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Approved as to style and content by:

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Gerard Coté	Edward A. Funkhouser
(Fellows Advisor)	(Executive Director)

April 2006

Major: Biomedical Engineering

ABSTRACT

Detection of Physiologically Relevant Alcohol Concentrations Using Raman Spectroscopy (April 2006)

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Fellows Advisor: Dr. Gerard Coté
Department of Biomedical Engineering

This is the first step in a series of studies to test the feasibility of using Raman Spectroscopy (RS) to non-invasively detect physiologically relevant blood alcohol concentrations. Blood tests, urine tests, and the breathalyzer are currently the most commonly used techniques to measure blood alcohol content. Blood tests are invasive and require wet labs. Although urine tests are non-invasive, they also require wet labs. The breathalyzer is non-invasive and does not require a lab, but its accuracy has come into question. This method measures alcohol content in the alveolar air, which is not always a reliable predictor of alcohol content in the blood. A Raman-based technique could alleviate these problems and eventually replace or complement the breathalyzer.

To explore this option, samples of ethanol-in-water from 0-1.0% (wt/vol) were prepared, and a time study was performed to test both the ability of RS to detect alcohol in relatively short amounts of time and to find an optimum scanning time. The spectra were used to create a partial least squares (PLS) model, which uses differences in the spectra to construct a model to describe the relationship between certain peaks and alcohol concentration. The model was used to predict the concentration of several known samples. The accuracy of the model's prediction was compared for each stage of the time study. This study then focused on measuring ethanol concentrations in plasma, a much more complicated media than water. Again, a model was constructed, used to predict alcohol concentrations, and tested for accuracy. This study showed that Raman spectroscopy has the ability to detect alcohol in the physiological range in rather complex environments and in limited time windows, but repeatability is the main question. Spectra have a tendency to be inconsistent at such low alcohol concentrations, which results in a weak model and less accurate predictions.

I would like to dedicate this thesis to my friends and family for their continued love and support through good times and bad. Without my friends and family, I would not have had many of the opportunities and accomplishments that I have, including this project and thesis.

ACKNOWLEDGEMENTS

The experiences I have gained while working on this project and writing this thesis have been immeasurable. It has been somewhat of a roller coaster ride, but all the long hours, frustration, and late nights have been worth it. I will draw upon these times even after I have left this lab and University. None of this would have been possible without the help of many individuals and I would like to take the time to thank them for their efforts.

First and foremost I would like to thank my family. They have supported me in all my endeavors and, in doing so, sacrificed valuable time, money, and patience. Everything I am, I owe to them.

I would also like to thank Dr. Gerard Coté and all the other members of the Optical Bio-Sensing Lab. Without Dr. Coté allowing me the opportunity to participate in the Fellows program, this thesis would not have been possible. He provided countless resources and time, and for that I'm grateful. The other members of the lab were also essential to the progress of this project, especially Bennett and Angela. Their guidance, willingness to answer any and all questions, and help with all the steps along the way have not been overlooked or taken for granted. Everyone in the lab has been friendly

and kind since day one. I will certainly miss our daily lunches and other social activities. So I say thank you and wish the best to Bennett, Angela, Hope, Becky, Lee, Brandon, Janie, and Ethan.

Finally I would like to thank the Office of Honors Programs and Academic Scholarships for the funding support they provided and everyone involved in the Fellows program, specifically Mrs. Jennifer Veracruz and Mrs. Cindy Raisor. This is a unique and valuable opportunity that many students across the country are never offered. It takes a solid core of people to put a program of this nature together and keep it running smoothly through all the difficulties that research can bring. You have all done a great job and I encourage you to keep up the good work.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

INTRODUCTION[1]

Thousands of people are killed each year in the United States due to alcohol related traffic accidents. To combat this problem, law enforcement agencies impose harsh penalties and high fines on people who are convicted of driving drunk. The techniques that are currently used for testing a driver's blood alcohol content (BAC) are not completely adequate or ideal though. Because of this, some drivers are not being punished for driving while intoxicated. The purpose of this project is to try and overcome the drawbacks of the techniques that are currently used by developing a Raman Spectroscopy (RS) based technique to measure BAC directly and non-invasively. A RS-based technique could be used in field sobriety tests to help combat drunk driving and decrease fatalities due to alcohol-related traffic accidents. This study, however, seeks to determine if RS can detect alcohol at physiological levels in limited time windows and then in rather complicated media such as plasma.

It has been shown in previous studies that RS can be used to detect various biological compounds, including ethanol. The majority of these studies are done at much higher concentrations than what are found in physiological systems, however.

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[1] This thesis follows the style and format of *Journal of Biomedical Optics.*

Further studies to test the ability of RS to detect ethanol at physiological concentrations were needed. These necessary experiments were performed in this study and showed that while RS is capable of detecting ethanol at physiological concentrations in both water and plasma, repeatability is a concern. The low concentrations and short integration times increase the variability between experiments. The ability of RS to consistently detect ethanol at such low concentrations in water and plasma was not apparent from this study and must be further investigated before any additional experiments should be performed.

PROBLEM

BACKGROUND INFORMATION

Current Techniques for Measuring Blood Alcohol

The Fatality Analysis Reporting System maintained by the National Traffic Highway Safety Administration reveals that there are approximately 17,000 people killed each year in the United States in alcohol related traffic accidents. This total makes up approximately 40% of all traffic fatalities that occur in the U.S. each year.[1] In order to combat this problem, law enforcement officials impose tough penalties on those that are convicted of driving drunk. These penalties include jail time, fines, and suspension of license. In the U.S., the legal blood alcohol limit for drivers is 0.08% wt/vol (0.08% of the weight of the blood consists of alcohol).[2] The law enforcement officials require a device that can quickly and accurately measure a driver's blood alcohol content (BAC) to enforce these laws.

The three most popular techniques to test BAC are blood tests, urine tests, and breathalyzers. A blood test is a highly accurate technique for measuring BAC, but is invasive and requires a wet lab with skilled technicians. Although they are non-invasive,

urine tests also require a wet lab with skilled technicians. The breathalyzer is currently the most popular technique for field BAC tests. The accuracy of the breathalyzer has recently been brought into question, however.[3] Small amounts of alcohol in the blood are passed into the alveoli in the lungs, where it is then expired. The breathalyzer measures the alcohol content of the expired air and uses these levels to predict BAC. However, alcohol in the mouth and throat may mix with expired air, causing a person to test positive for higher BAC levels than are actually present. Because it is only the alcohol in the blood that eventually reaches the brain and causes impaired judgment and motor function, there is a need for a test that measures BAC more directly, but is still portable and non-invasive.

Raman Spectroscopy

Raman Spectroscopy is based on the Raman scattering of light from a molecule of interest. When light hits a molecule, a small percentage of the light is inelastically scattered. This means that the energy content of the light scattered from the molecule is not identical to the energy of the light that initially hit the molecule. The magnitude of this shift in the energy content is highly dependent on the type of bonds present in the molecule and corresponds to a peak in the spectrum. The Raman spectrum of a

molecule is very unique, and thus, RS can be used as a detection technique. The high selectiveness makes RS an ideal technique to detect various biological molecules, pharmaceuticals, and other drugs in solutions containing many other chemicals. It has already been shown that various molecules and substances including albumin, glucose, urea, cholesterol, and triglyceride can be detected in solution by RS.

LITERATURE REVIEW

Detection Using Raman Spectroscopy

Many studies have attempted to use RS to detect various analytes in solution. There are several key factors that affect the results of these studies: the sampling time, the laser power, and the complexity of the solvent of the solution. For RS to really become an effective detection technique *in vivo*, it must be able to accurately predict very small concentrations in extremely complex solvents with low laser power and relatively short sampling time.

Initial Raman studies were aimed at proof of concept, and thus were performed in basic solutions of water, saline, etc. Initially, RS was shown to accurately measure concentrations of glucose, lactate, ascorbate, pyruvate, and urea in water solutions at

higher than physiological concentrations. To obtain these results, a 200-mW laser was used with a sampling time of 1 hour per sample.[4] This paved the way for more complex studies to be performed. For example, it was shown that glucose, lactic acid, and creatinine could also be accurately measured at much higher than physiological concentrations in saline solutions. These results required a 200-mW laser with a sampling time of 100 seconds per sample.[5]

With more promising results, the focus turned towards detection of analytes in whole blood. Again, these results showed great potential. Glucose concentrations were determined in whole blood at above-physiological levels. This study was performed with a 150-mW laser and a sampling time of 5 minutes per sample.[6] Whole blood adds many more complications due to the red blood cells. For example, glucose is lost at a rate of about 6% per hour at room temperature.[6] This makes detection and prediction of concentrations a two-step process: the actual measurements and then the correction due to component loss. The whole blood studies have been repeated many times and expanded to include physiological concentrations of glucose, cholesterol, urea, albumin, and triglyceride with a 250-mW laser and 60 second sampling time.[7]

Detection of Alcohol Using Raman Spectroscopy

Using RS to characterize alcohol in solution has not been studied in as much depth as some other compounds, but initial studies have shown positive results. Higher than physiological concentrations of ethanol could be detected in deionized water using a 300-mW laser and a sampling time of 1-5 minutes per sample.[8] Additionally, the concentration of ethanol in an oral liquid was determined using RS. This study detected the ethanol content through an amber plastic bottle, which is more difficult to detect through than a clear cuvette or vial.[9]

METHODS

All Raman spectra were collected using a Raman Systems R-3000 Raman Spectrometer (Ocean Optics Dunedin, FL) with a 785 nm high power laser delivering 500-mW to the sample. A significant amount of the laser power was lost within the spectrometer, so the actual measured power delivered to the sample was 320-mW. Although the goal of this project is to investigate whether the commercial Raman spectrometer can measure physiologically relevant blood alcohol concentrations, the initial experiments were performed with ethanol dissolved in spectroscopy-grade water. This is because blood is a very complex media and would cause many unnecessary complications in the early stages of the study.

An initial time study was conducted to test the effect that the integration time had on the system's ability to detect ethanol. A 1.0% (wt/vol) stock solution of pure ethanol (Sigma St. Louis, MO) in spectroscopy-grade water (Sigma St. Louis, MO) was prepared. A predetermined amount of the solution was placed into a glass vial and diluted to 3 ml using spectroscopy-grade water. Each sample was prepared separately, using the same dilution technique and allowed to sit for at least 30 minutes before being placed into the spectrometer.

When collecting the Raman spectrum of each sample, the entire vial was placed into the sample holder and the laser was then placed against the vial with the liquid spacer in place. The order of the samples was randomized and non-consecutive triplicates of each sample were taken. The integration time, or time required to obtain a Raman spectrum for each sample, was varied for each complete set of triplicates. The integration times selected were 5, 10, 15, 30, 60, and 120 seconds.

All data processing was performed using MATLAB 7.1 (Mathworks, Inc) and the MATLAB PLS Toolbox 3.0 (Eigenvector Research Incorporated). The MATLAB code is included in the Appendix. The data for each complete set of triplicates was organized into two groups: calibration and prediction. Table 1 shows the concentrations of the samples selected for each group.

Table 1. Selected Concentrations for Calibration and Prediction Data Groups
(all data collected in triplicates)

	Calibration Data Set	**Prediction Data Set**
Concentrations of Samples (% wt/vol)	0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50 0.55 0.60 0.65 0.70 0.75 0.80 0.85 0.90 0.95 1.0	0.035 0.065 0.075 0.085 0.17 0.41 0.73

The calibration data consisted of 29 triplicates (87 total spectra) and was used to construct the PLS model. The prediction data consisted of 7 triplicates (21 total spectra) and was not included when building the PLS model. Instead, this data was input into the model, and the model was used to predict the concentration of each prediction sample. Each triplicate point was averaged for the prediction and calibration data to account for variability between sets. The data for each integration time was then compared and the integration time that yielded the model with the best predictive capability was selected.

The next part of this study focused on measuring ethanol in plasma, a simpler media than blood but more complex than water. Bovine blood (Veterinary School, Texas A&M University) was placed in a centrifuge for 15 minutes at 3500 rpm to separate the red blood cells from the plasma. After isolating the plasma, again a 1.0% (wt/vol) stock solution was prepared. Samples of the same concentrations were made from the stock solution according to the previously mentioned procedure. The data was collected using only the integration time selected from the previous time study. The data analysis was conducted in the same manner.

RESULTS

The first step in the time study, the PLS model of the data collected with a 5-second integration time, is shown in Figure 1. Fig. 1 (a) shows the entire range for both the calibration and prediction group. The calibration data was used to construct the PLS model. This model was then used to interpret the prediction data and predict the concentration of each sample. In theory, all the data points should lay on a line in a 1:1 (predicted vs. actual) manner, meaning that what the model predicts for the sample's concentration is the actual concentration of the sample. Fig. 1 (a) shows that, while the model appears to have a strong correlation between predicted and actual concentrations for the calibration set, it cannot accurately predict the concentrations of the prediction data samples. The accuracy of the model and the inaccuracy of prediction are most likely because the model is constructed using information that is not indicative of the presence of alcohol. In other words, the model is using too much of each spectrum to model the presence of alcohol. It is possible that the short integration time doesn't supply enough characteristic information about the alcohol in solution to result in an accurate prediction by the model. Fig. 1 (b) shows just the physiological range of the model. The higher concentrations of alcohol are necessary to make the model accurate,

but are not the regions of interest for this study. The physiological range clearly shows that the model's predictions are not accurate. In some cases, the model even predicts concentrations that are nearly 6 times greater than actually present.

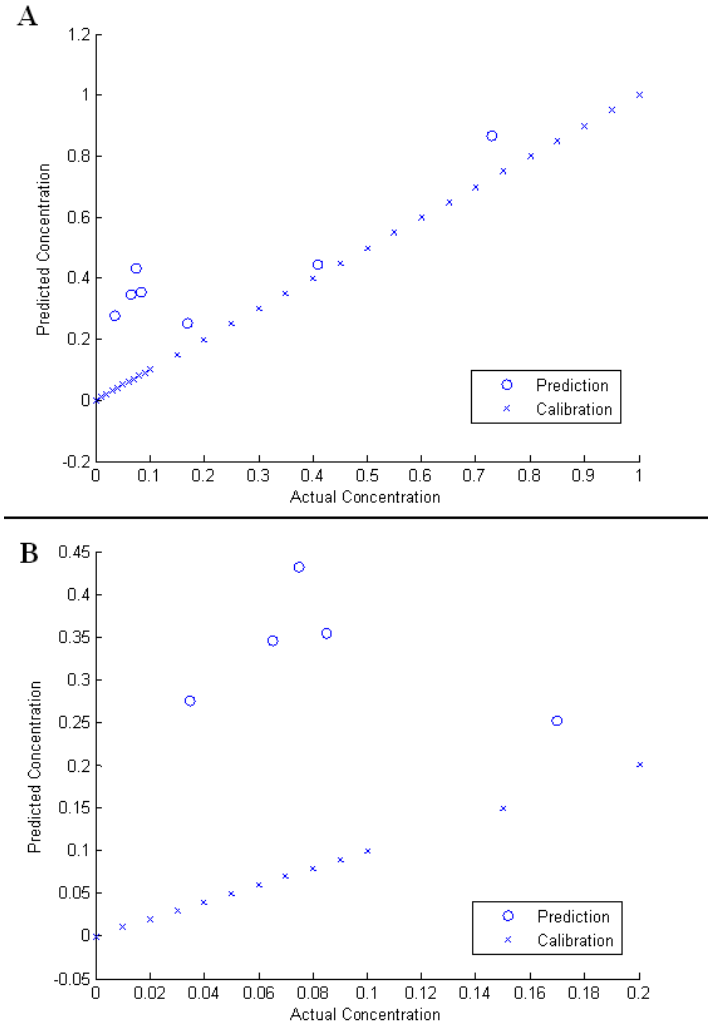

Figure 1. PLS Model of Ethanol-in-Water Data Collected with 5-second Integration Time. ((a) Full range of model, (b) Physiological range of model)

Figure 2 shows the PLS model constructed with the 10-second data. Again, Fig. 2 (a) shows the entire range for both the calibration and prediction group, while Fig. 2 (b) shows just the physiological range. Similar to the model of the 5-second data, this model appears to have a strong correlation between predicted and actual concentrations but cannot accurately predict the concentrations of the prediction data. The predictions, however, are more accurate in this model. The greatest prediction error in the physiological range appears to only be about 3 times the concentration that is actually present.

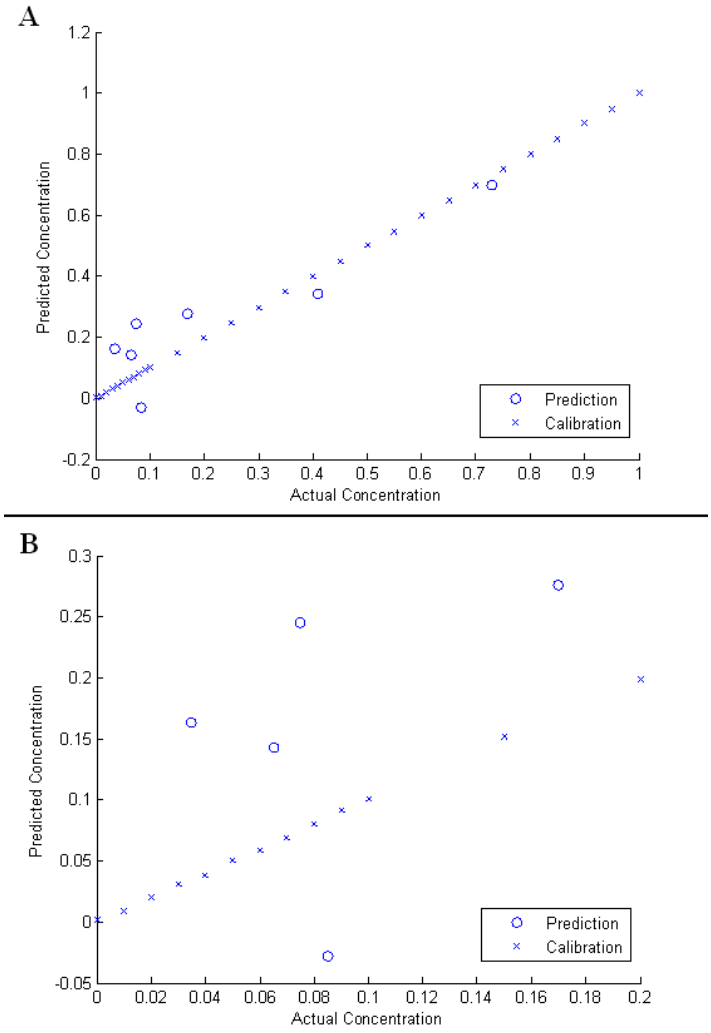

Figure 2. PLS Model of Ethanol-in-Water Data Collected with 10-second Integration Time ((a) Full range of model, (b) Physiological range of model)

Figure 3 shows the PLS model constructed with the 15-second data. This model shows improved results when compared to the model of the 10-second data. Although only minor improvements can be seen in the maximum error when predicting the

concentration of the prediction samples, it is clear that the predictions are more accurate overall. In general, the prediction points lie closer to the line representing the model.

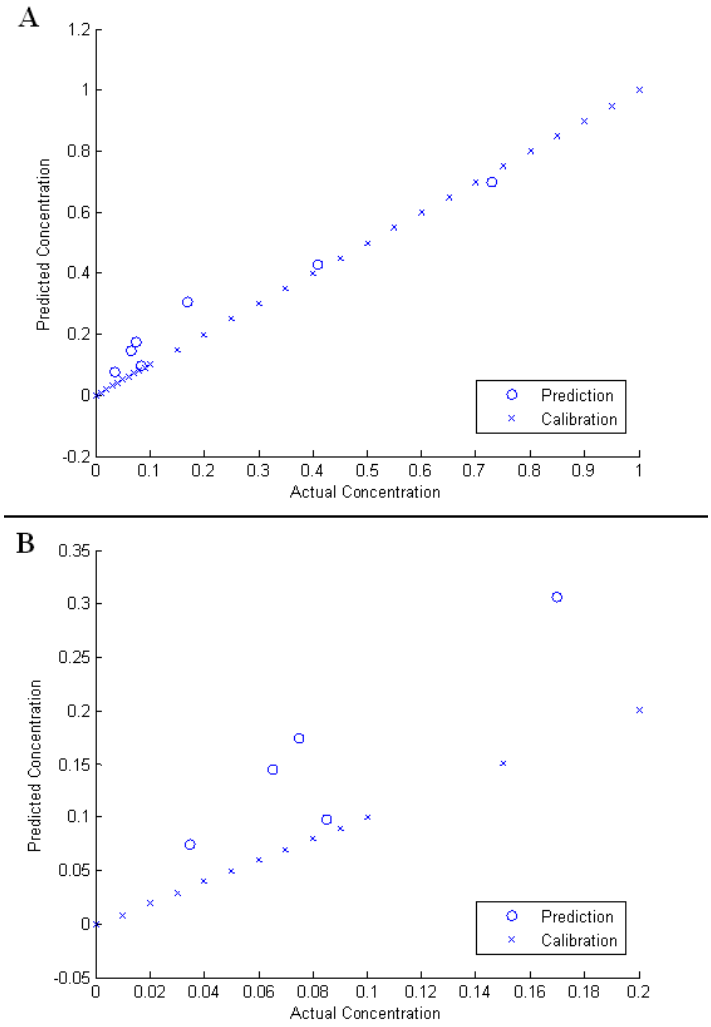

Figure 3. PLS Model of Ethanol-in-Water Data Collected with 15-second Integration Time ((a) Full range of model, (b) Physiological range of model)

Figure 4 shows the next stage in the time study, the PLS model of the data collected with a 30-second integration time. Again, there doesn't seem to be any major improvement in the maximum error when predicting the concentrations of the prediction samples, but the overall predictive abilities of the model are improved. Two of the prediction points in the physiological range appear to be accurate, while the others are still located around the model line. At this stage, it is still safe to assume that the model is using information that is not really an indicator of alcohol to predict concentrations because of the highly accurate model but inaccurate predictions.

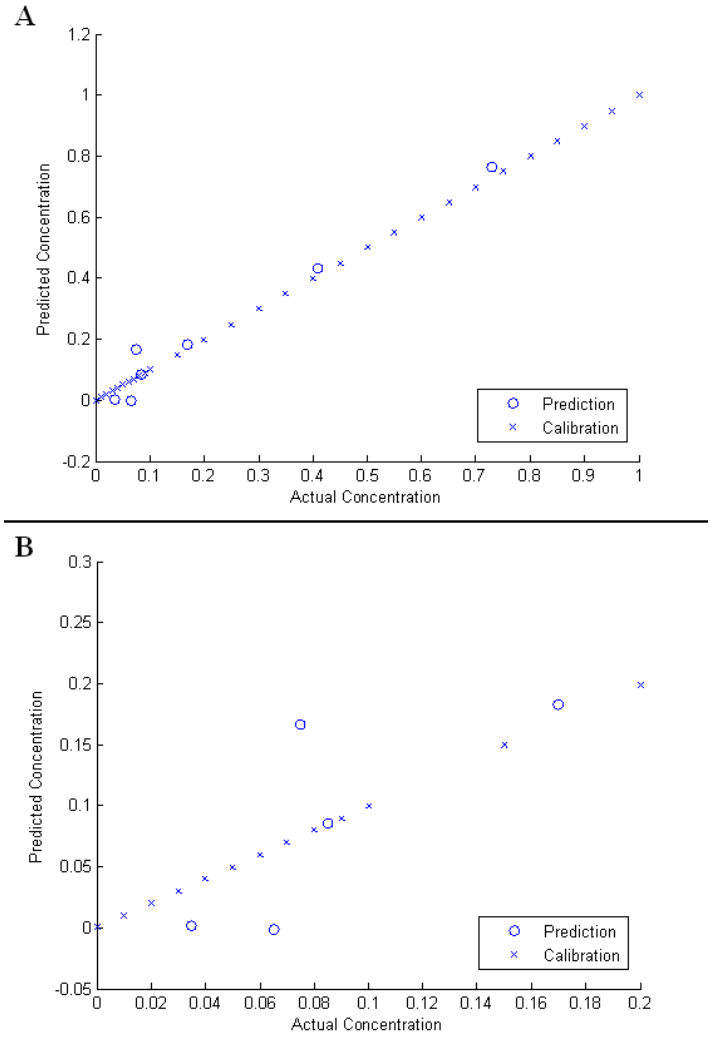

Figure 4. PLS Model of Ethanol-in-Water Data Collected with 30-second Integration Time ((a) Full range of model, (b) Physiological range of model)

The PLS model constructed with the 60-second data is shown in Figure 5. This model again shows improvements over the data collected with the shorter integration time before it. There is only one prediction point that might be considered accurate, but as a whole it can be seen that the points are more consistent around the line. The

prediction points are more correlated with each other. One concentration is not grossly over-predicted while the next is under-predicted. This shows a more representative model. Also, the maximum error in prediction appears to have decreased. The model itself is not as accurate as the previous data sets, especially in the physiological range. This is expected, however, because now it can be hypothesized that the model is using parts of each spectrum more selectively. Mostly, the parts corresponding to just alcohol are being drawn upon to construct the model. Because the prediction points and the model are showing similarities in error, the error is assumed to be more because of the difficulty in detecting such small amounts of alcohol in solution, rather than the lack of characteristic information in the spectra.

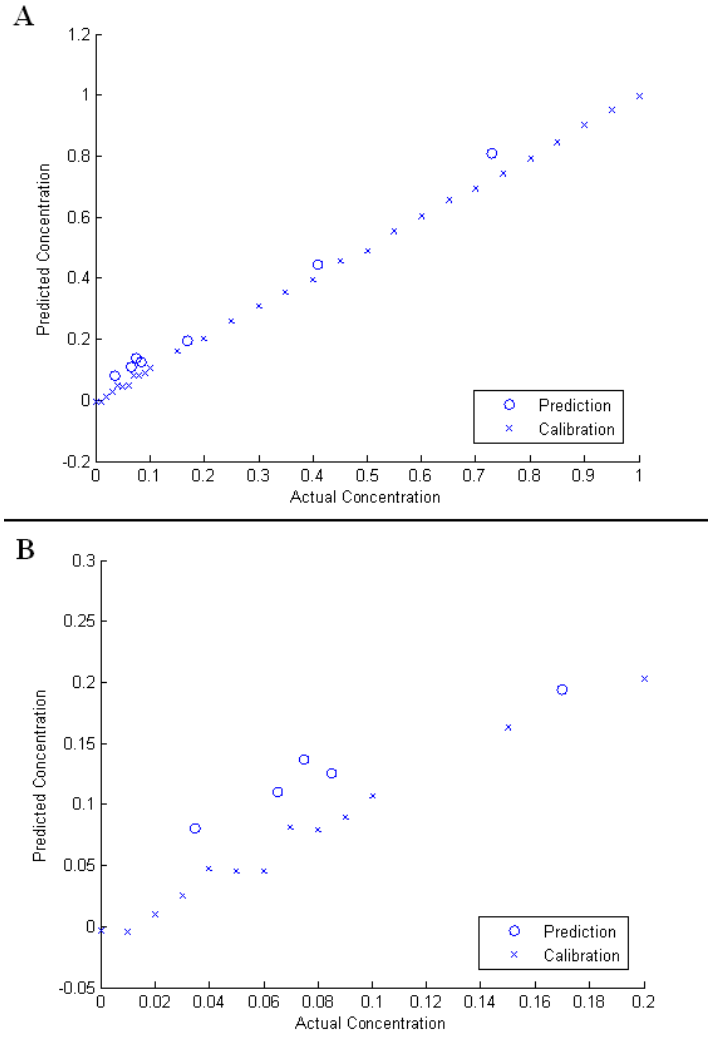

Figure 5. PLS Model of Ethanol-in-Water Data Collected with 60-second Integration Time ((a) Full range of model, (b) Physiological range of model)

Figure 6 shows the final step of the time study, the PLS model of the data collected with a 120-second integration time. This model shows some error in calibration, similar to the model of the 60-second data. This shows that again the model is more representative of the solution than any of the models of data collected with

shorter integration times. This model is the most accurate at predicting the concentrations of the prediction samples. Both the maximum error in prediction and the consistency of the predictions are the best out of all the other models.

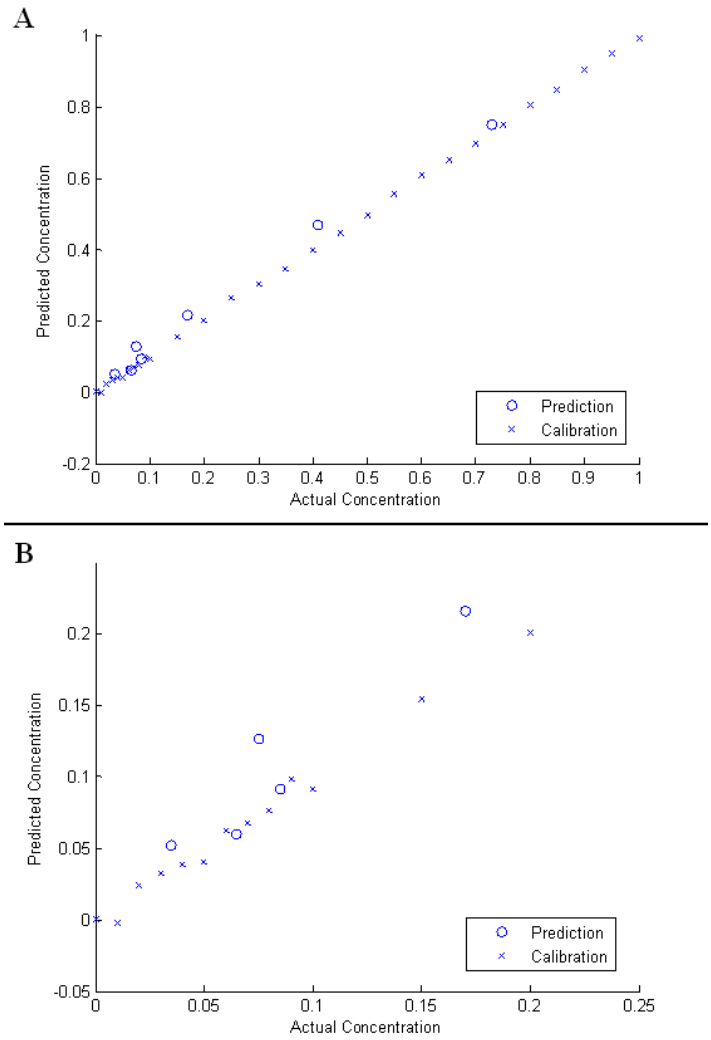

Figure 6. PLS Model of Ethanol-in-Water Data Collected with 120-second Integration Time ((a) Full range of model, (b) Physiological range of model)

Table 2 shows the error of prediction for the model created using the data of each step in the time study. This shows that the 120-second integration time should produce the best results for any future work with this spectrometer. Although it might be beneficial to increase the integration time even higher than 120-seconds, the spectrometer used in this project cannot exceed this time. Additionally, an integration time much longer than 120-seconds would not be realistic for a field sobriety test, the eventual goal of this project.

Table 2. Error of Prediction for Time Study Data Sets

Integration Time of Data Set	**Error**
5 Seconds	283%
10 Seconds	135%
15 Seconds	64.2%
30 Seconds	46.9%
60 Seconds	45.8%
120 Seconds	27.5%

Figure 7 shows the PLS model of ethanol-in-plasma data collected with a 120-second integration time. As expected, the model's ability to predict concentrations does not appear to be as accurate as when ethanol is dissolved in water. Plasma can contain proteins, salts, sugars, enzymes, lipids, and many other biological components, and thus,

is a much more complicated media than water. The model is still comparable, however, with the ethanol-in-water model. Two of the predicted points in the physiological range lie within the region of the model. One predicted concentration is dramatically less than what is actually present, but again, any one of the additional components of plasma could have caused these problems. Table 3 shows the error of prediction for the ethanol in water and the ethanol in plasma data sets taken with a 120 second integration time. This shows that the additional components of the plasma made it more difficult to predict concentrations.

Table 3. Error of Prediction for Water and Plasma Data with 120 Second Integration Time

Solution with Ethanol	**Error**
Water	27.5%
Plasma	35.3%

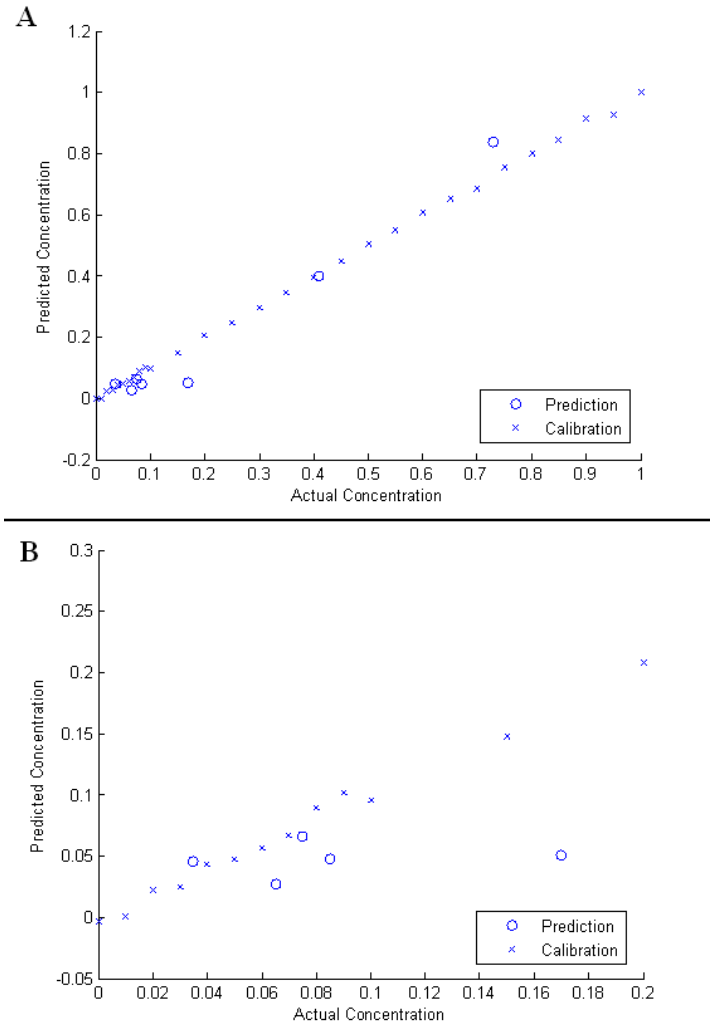

Figure 7. PLS Model of Ethanol-in-Plasma Data Collected with 120-second Integration Time ((a) Full range of model, (b) Physiological range of model)

SUMMARY AND CONCLUSIONS

SUMMARY OF STUDY

The time study that was performed with samples of ethanol dissolved in water showed somewhat expected results. The ability of the model to accurately predict the concentrations of the prediction samples improved as the integration time, or time spent acquiring each spectrum, increased. This resulted in the 120-second integration time data producing the best model at prediction.

It should also be noted that the data collected with integration times less than about 30-seconds appeared to create models that represented the calibration data very accurately but could not give accurate predictions. This is assumed to happen because the model was using too much of each spectrum to characterize the alcohol in solution. The data collected with shorter integration times do not contain enough information to effectively characterize the alcohol in solution, so when used to construct a model, it is unable to accurately predict alcohol concentrations.

The plasma study showed promising results. Despite the plasma being a much more complicated media than water, the model was still relatively accurate in predicting the concentrations of most of the prediction samples. The predictive capabilities of the

model should not be expected to be equal to or exceed the accuracy of the ethanol-in-water model because of the difference in media.

CONCLUSIONS

The purpose of this study was to further the knowledge of using Raman Spectroscopy to detect alcohol, specifically at physiological concentrations, with the eventual goal of developing a non-invasive, Raman-based blood alcohol detector. The primary concerns that were investigated were if such low levels of alcohol could be detected in water and plasma, a more complicated medium, with a limited time window.

The time study that was performed showed that ethanol could be measured at physiological levels in a limited time window. Theoretically, the more time that is allowed to acquire each spectrum, the more accurate the detection will be. With the eventual goal of developing a blood-alcohol detector, it must be kept in mind that allowing much more than a few minutes per spectrum is unreasonable. A smaller time window must be used to make the findings more applicable towards the goal of the overall project. This was accomplished when a model was shown to be able to reasonably predict alcohol concentrations with data that was collected with 120-second integration times. Ideally, the integration time would be even further reduced, but this

study was aimed at testing the feasibility of the reduced time. From here, more studies may be conducted to test the capabilities of measuring physiological alcohol concentrations in reduced time windows and more complicated media. Time studies may be performed in other media such as urine, plasma, or whole blood.

The aim of trying to measure physiological levels of alcohol in a complicated media like plasma proved to be more troubling. The many components contained in the plasma added interference and noise to the detection measurements. This is believed to be one of the main reasons why the prediction of the model is not as accurate as the ethanol-in-water model. The model, however, still showed some promising results. Further studies need to be performed to better characterize the ability of RS to measure alcohol in complicated media like plasma.

The main issue that consistently came up when using RS to measure physiological levels of alcohol was repeatability. Because these are such low concentrations and a limited time window is in use, there is a high variability between data sets. This also causes problems in model calibrations, especially in plasma. As the plasma is allowed to sit, components of the plasma begin to fall out of solution. This leads to changes in the spectra of the samples and reduces the model's ability to predict

samples over time. Although this study shows that RS is capable of measuring alcohol at physiological levels, it does not address the repeatability issues. More studies that characterize the ability to measure these levels of alcohol consistently over time should be performed before additional experiments are explored.

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APPENDIX

```
clear;
clc;
clf;

matrix1(:,1) = csvread('WAT1201_0026.csv',10,1);
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matrix1(:,22) = csvread('WAT1201_0011.csv',10,1);
matrix1(:,23) = csvread('WAT1201_0022.csv',10,1);
matrix1(:,24) = csvread('WAT1201_0001.csv',10,1);
matrix1(:,25) = csvread('WAT1201_0035.csv',10,1);
matrix1(:,26) = csvread('WAT1201_0017.csv',10,1);
matrix1(:,27) = csvread('WAT1201_0006.csv',10,1);
matrix1(:,28) = csvread('WAT1201_0036.csv',10,1);
matrix1(:,29) = csvread('WAT1201_0021.csv',10,1);
matrix1 = matrix1(400:2047,:);
```

```
matrix2(:,1) = csvread('WAT1202_0012.csv',10,1);
matrix2(:,2) = csvread('WAT1202_0030.csv',10,1);
matrix2(:,3) = csvread('WAT1202_0004.csv',10,1);
matrix2(:,4) = csvread('WAT1202_0015.csv',10,1);
matrix2(:,5) = csvread('WAT1202_0036.csv',10,1);
matrix2(:,6) = csvread('WAT1202_0005.csv',10,1);
matrix2(:,7) = csvread('WAT1202_0019.csv',10,1);
matrix2(:,8) = csvread('WAT1202_0022.csv',10,1);
matrix2(:,9) = csvread('WAT1202_0029.csv',10,1);
matrix2(:,10) = csvread('WAT1202_0009.csv',10,1);
matrix2(:,11) = csvread('WAT1202_0016.csv',10,1);
matrix2(:,12) = csvread('WAT1202_0027.csv',10,1);
matrix2(:,13) = csvread('WAT1202_0001.csv',10,1);
matrix2(:,14) = csvread('WAT1202_0024.csv',10,1);
matrix2(:,15) = csvread('WAT1202_0011.csv',10,1);
matrix2(:,16) = csvread('WAT1202_0033.csv',10,1);
matrix2(:,17) = csvread('WAT1202_0003.csv',10,1);
matrix2(:,18) = csvread('WAT1202_0032.csv',10,1);
matrix2(:,19) = csvread('WAT1202_0014.csv',10,1);
matrix2(:,20) = csvread('WAT1202_0035.csv',10,1);
matrix2(:,21) = csvread('WAT1202_0018.csv',10,1);
matrix2(:,22) = csvread('WAT1202_0008.csv',10,1);
matrix2(:,23) = csvread('WAT1202_0023.csv',10,1);
matrix2(:,24) = csvread('WAT1202_0017.csv',10,1);
matrix2(:,25) = csvread('WAT1202_0006.csv',10,1);
matrix2(:,26) = csvread('WAT1202_0028.csv',10,1);
matrix2(:,27) = csvread('WAT1202_0002.csv',10,1);
matrix2(:,28) = csvread('WAT1202_0021.csv',10,1);
matrix2(:,29) = csvread('WAT1202_0026.csv',10,1);
matrix2 = matrix2(400:2047,:);

matrix3(:,1) = csvread('WAT1203_0013.csv',10,1);
matrix3(:,2) = csvread('WAT1203_0025.csv',10,1);
```

```
matrix3(:,3) = csvread('WAT1203_0020.csv',10,1);
matrix3(:,4) = csvread('WAT1203_0033.csv',10,1);
matrix3(:,5) = csvread('WAT1203_0003.csv',10,1);
matrix3(:,6) = csvread('WAT1203_0029.csv',10,1);
matrix3(:,7) = csvread('WAT1203_0017.csv',10,1);
matrix3(:,8) = csvread('WAT1203_0008.csv',10,1);
matrix3(:,9) = csvread('WAT1203_0035.csv',10,1);
matrix3(:,10) = csvread('WAT1203_0021.csv',10,1);
matrix3(:,11) = csvread('WAT1203_0028.csv',10,1);
matrix3(:,12) = csvread('WAT1203_0015.csv',10,1);
matrix3(:,13) = csvread('WAT1203_0005.csv',10,1);
matrix3(:,14) = csvread('WAT1203_0030.csv',10,1);
matrix3(:,15) = csvread('WAT1203_0012.csv',10,1);
matrix3(:,16) = csvread('WAT1203_0027.csv',10,1);
matrix3(:,17) = csvread('WAT1203_0010.csv',10,1);
matrix3(:,18) = csvread('WAT1203_0019.csv',10,1);
matrix3(:,19) = csvread('WAT1203_0006.csv',10,1);
matrix3(:,20) = csvread('WAT1203_0034.csv',10,1);
matrix3(:,21) = csvread('WAT1203_0011.csv',10,1);
matrix3(:,22) = csvread('WAT1203_0022.csv',10,1);
matrix3(:,23) = csvread('WAT1203_0018.csv',10,1);
matrix3(:,24) = csvread('WAT1203_0002.csv',10,1);
matrix3(:,25) = csvread('WAT1203_0014.csv',10,1);
matrix3(:,26) = csvread('WAT1203_0036.csv',10,1);
matrix3(:,27) = csvread('WAT1203_0004.csv',10,1);
matrix3(:,28) = csvread('WAT1203_0024.csv',10,1);
matrix3(:,29) = csvread('WAT1203_0031.csv',10,1);
matrix3 = matrix3(400:2047,:);

Conc = [0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.15 0.2
0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95
1.0];

for i = 1:29
```

```
        matrixAverage(:,i) = (matrix1(:,i) + matrix2(:,i) +
matrix3(:,i))./3;
end

options = pls('options');
options.display = 'on';
options.plots   = 'final';
pre = preprocess('default','mean center');
options.preprocessing{1} = pre;   %
options.preprocessing{2} = pre;   %y-block

Conc = Conc';
matrixAverage = matrixAverage';
model = pls(matrixAverage,Conc,5,options);
temp = model.pred;
ModelData = cell2array(temp(2));

%*****************************************************PRED************
matrix1p(:,1) = csvread('WAT1201_0025.csv',10,1);
matrix1p(:,2) = csvread('WAT1201_0015.csv',10,1);
matrix1p(:,3) = csvread('WAT1201_0007.csv',10,1);
matrix1p(:,4) = csvread('WAT1201_0033.csv',10,1);
matrix1p(:,5) = csvread('WAT1201_0002.csv',10,1);
matrix1p(:,6) = csvread('WAT1201_0027.csv',10,1);
matrix1p(:,7) = csvread('WAT1201_0012.csv',10,1);
matrix1p = matrix1p(400:2047,:);

matrix2p(:,1) = csvread('WAT1202_0020.csv',10,1);
matrix2p(:,2) = csvread('WAT1202_0007.csv',10,1);
matrix2p(:,3) = csvread('WAT1202_0013.csv',10,1);
matrix2p(:,4) = csvread('WAT1202_0034.csv',10,1);
matrix2p(:,5) = csvread('WAT1202_0025.csv',10,1);
matrix2p(:,6) = csvread('WAT1202_0010.csv',10,1);
matrix2p(:,7) = csvread('WAT1202_0031.csv',10,1);
```

```
matrix2p = matrix2p(400:2047,:);

matrix3p(:,1) = csvread('WAT1203_0016.csv',10,1);
matrix3p(:,2) = csvread('WAT1203_0009.csv',10,1);
matrix3p(:,3) = csvread('WAT1203_0007.csv',10,1);
matrix3p(:,4) = csvread('WAT1203_0026.csv',10,1);
matrix3p(:,5) = csvread('WAT1203_0023.csv',10,1);
matrix3p(:,6) = csvread('WAT1203_0001.csv',10,1);
matrix3p(:,7) = csvread('WAT1203_0032.csv',10,1);
matrix3p = matrix3p(400:2047,:);

for i = 1:7
        matrixP(:,i) = (matrix1p(:,i) + matrix2p(:,i) +
matrix3p(:,i))./3;
end

PredConc = [0.035 0.065 0.075 0.085 0.17 0.41 0.73];
PredConc = PredConc';
matrixP = matrixP';

Predict = pls(matrixP, model,options);
temp = Predict.pred;
Prediction = cell2array(temp(2));
figure(99);
hold on
plot(PredConc, Prediction,'o');
plot(Conc, ModelData,'x');
hold off
```

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EDUCATION:

Texas A&M University
College Station, TX
Expected Graduation: May 2006

Bachelor's of Science Degree
Major: Biomedical Engineering
GPR: 3.76

RESEARCH EXPERIENCE:

Texas A&M University Undergraduate Research Fellows Program Class of 2006

- Thesis: *Detection of Physiologically Relevant Alcohol Concentrations Using Raman Spectroscopy*
- Investigating a more direct and non-invasive technique of measuring blood-alcohol concentrations in Dr. Gerard Coté's Optical Bio-Sensing Laboratory.

Texas A&M University Psychoneuroimmunology Lab

- Student worker from May 2004 to May 2005.
- Performed experiments for projects involving Theiler's virus, which is a mouse model for multiple sclerosis.
- Skills: Dissections, perfusions, IP injections, cannulae surgeries, bleeds, animal handling

HONORS AND AWARDS:

- Recipient of McFadden Scholarship
- Dean's List for the College of Engineering – 3 Semesters
- National Society of Collegiate Scholars Inductee
- Member of The National Dean's List
- Recipient of the 2004 Biomedical Engineering FMDIC Outstanding Junior Scholarship Award
- Recipient of an Undergraduate Summer Research Grant (USRG) from the Dwight Look College of Engineering at Texas A&M University (2005)

LEADERSHIP / ORGANIZATIONS

- One of 50 freshmen selected for L.I.F.E. (Leaders in Freshman Engineering) (2002-03)
- One of 30 students selected for Honors Student Council (2003-Present)
- Elected Vice President of Development for Honors Student Council (2004-Present)
- Alpha Epsilon Delta (Pre-medical Honor Society)
- Tau Beta Pi (Engineering Honor Society)
- Alpha Eta Mu Beta (Biomedical Engineering Honor Society)