Raman Analyzer for Illicit Drugs (RAID)

Group 2

Nicole Parker	Optical Engineer
Michael Soto	Optical Engineer
Asha Waters	Computer Engineer
Jean Georges	Computer Engineer

REVIEWERS:

Dr. Leland Nordin

Dr. Patrick LikamWa

Dr. Peter J. Delfyett

Dr. Azadeh Vosoughi

SPONSORS:

MKS Newport

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1 Executive Summary

In this paper, we discuss how Raman spectroscopy can be used to determine the presence of illicit substances in beverages. Raman spectroscopy operates on the principle of Raman scattering, a phenomenon where light interacts with molecular vibrations within a sample, leading to shifts in the wavelength of scattered light. When a laser is directed at a sample, most of the light is elastically scattered without changing its wavelength (Rayleigh scattering), but a small fraction undergoes inelastic scattering due to interactions with molecular vibrations of the sample's molecules, resulting in a change of the lights wavelength (Raman scattering). This change, or shift, is unique to the molecular structure of the substance and thus acts like a molecular fingerprint. By analyzing these shifts with a spectrometer, it is possible to identify the presence of specific molecules, including drugs. Each drug has a unique Raman spectrum, enabling the precise identification of substances within a complex mixture without the need for direct contact or sample preparation. This makes Raman spectroscopy a powerful tool for identification of drugs for public safety.

This innovative device provides a safe and effective way to detect a compromised beverage. GHB (gamma-hydroxybutyric acid), ketamine and Rohypnol are the most common "date-rape" drugs and ideally would be what the spectrometer should detect. However, these substances are scheduled III drugs and are not allowed to be handled for school projects. For demonstration purposes, instead of identifying the aforementioned drugs, the substance that will be identified with our device, Raman Analyzer for Illicit Drugs (RAID), is Gamma-Aminobutyric acid (GABA). GABA is a naturally occurring amino acid that acts as a neurotransmitter in the brain and a nutritional supplement. It is also a precursor to gamma-hydroxybutyric acid (GHB), a substance that has been misused as a recreational drug with potentially dangerous effects; it is often misused as a "roofie", a term referring to its illicit use to incapacitate individuals, typically in contexts of sexual assault.

Although GHB and GABA share some common structural elements, such as the carbon backbone and amine group, the presence of additional functional groups in GHB can introduce new vibrational modes and alter the overall spectral profile. Therefore, while there are likely to be discernible differences that allow for their differentiation using Raman spectroscopy, there may be some similarities in the Raman spectra of GHB and GABA due to their structural relationship. For this reason, GABA serves as a promising alternative to GHB for demonstrating the functionality of RAID.

The motivation behind developing a spectrometer to detect said substances in drinks stems from the alarming prevalence of drug-facilitated sexual assault incidents in America. According to the National Sexual Violence Resource Center (NSVRC), approximately 1 in 5 women and 1 in 71 men in the United States

have experienced rape at some point in their lives. Furthermore, the Substance Abuse and Mental Health Services Administration (SAMHSA) reports that drug-facilitated sexual assaults, where drugs are used to incapacitate victims, contribute significantly to the overall incidence of sexual assault.

Therefore, the development of a Raman spectrometer for the detection of GHB, and thus GABA, in liquid samples represents a significant technological advancement in ensuring the safety and well-being of individuals in social environments such as bars and clubs. Our team has developed a Raman spectrometer specifically designed for the rapid and accurate detection of GABA in various liquid samples. This device employs advanced spectroscopic techniques to identify the unique molecular fingerprint of GABA. With a focus on user-friendliness, the RAID spectrometer features an easy-to-navigate interface that enables non-expert users to operate the device with no training. RAID leverages a high-sensitivity detection system and sophisticated algorithms to analyze the Raman spectra of samples, enabling the identification of GABA. Its compact design and quick analysis make it an ideal solution for on-site testing in bars and clubs.

The primary application of RAID is in public venues such as bars and clubs, where it can be used to test drinks for the presence of misused substances in drinks. By providing a simple and effective method for testing substances on-site the device plays a crucial role in enhancing public safety and awareness. It empowers both business owners and patrons with the ability to verify the safety of beverages, contributing to a safer social environment.

In contrast to traditional Raman spectrometers, which often demand specialized expertise, complex sample preparation, and substantial investment, RAID distinguishes itself through its user-friendliness interface, cost-effectiveness, and rapid and accurate detection capabilities. Traditional methods for identifying the presence of substances in drinks typically rely on chemical test strips or dyes that change color in presence of specific drugs. While these solutions offer a straightforward approach, they come with limitations such as – versatility and scope, reusability, and economic and environmental impact – that RAID addresses and surpasses.

Building the Raman spectrometer capable of detecting desired substances in drinks involves comprehensive research into various key components. The optical subsystem requires careful consideration, focusing on high-quality light sources such as a laser with a wavelength of 532nm, for optimal substance identification. Photodetectors, capable of accurately capturing the reflected or transmitted light, are crucial for precise data acquisition. The microprocessor, a critical component, was chosen for its processing power and ability to handle complex algorithms involved in substance identification. Careful exploration of suitable materials for our project's construction, considering factors like durability, safety, and compatibility with different drink compositions, is vital. Thorough

research into each component is essential to ensure the spectrometer's efficacy, reliability, and user-friendliness.

The project developed a reliable and cost-effective spectrometer designed to detect GABA in lieu of GHB, with a particular focus on enhancing safety in social settings. The distinguishing feature lies in the dye-free method, ensuring the fluid remains safe for consumption. The microprocessor-driven system processes optical data efficiently, providing quick and reliable results. By combining research on optimal components, including precision optics, sensors, and robust algorithms, the project created an affordable, user-friendly solution that empowers individuals to proactively safeguard against drug-facilitated crimes in an accessible and non-intrusive manner.

We thank MKS Newport for sponsoring this project by supplying the necessary parts to build RAID.

2 Project Description

This project's main objective is to develop a Raman spectrometer designed for detecting substances in beverages. The user will interact with a touch screen to select the drink they are testing. The Raman spectrometer will then analyze the beverage and provide results in real-time.

This Raman spectrometer, named Raman analyzer for illicit drugs (RAID), utilizes a laser driver and a 532nm laser diode. (This wavelength was chosen for its efficiency in Raman scattering and compatibility with a wide range of substances.) This serves as the excitation source, illuminating the beverage and inducing a Raman effect – a shift in the frequency of scattered light, which is characteristic of the molecular composition of the substance in question. A collimating lens and notch filter may be necessary to filter the pump.

The beam will pass through a dichroic mirror, then focus onto a sample of GABA solution. Consequently, Raman and Rayleigh scattering occurs, and the light travels back towards the dichroic mirror. From the dichroic mirror, the light is reflected through a longpass filter to filter out the Rayleigh scattered light. The Raman spectrum is then focused by a lens into a multimode optical fiber. The collected light is then analyzed using a Czerny-turner spectrometer configuration. This setup is renowned for its high spectral resolution and accuracy, making it an ideal choice for the precise detection of various chemical compounds. The light will be spatially filtered then collimated by a lens. Using an electronic rotation stage, a grating will rotate to reflect each of the scattered wavelengths through a focusing lens and into a photodiode.

The electrical signals from the photodiode are processed, by a microcontroller, to extract the Raman spectrum, which is then compared against a pre-loaded spectrum of GABA. This comparison enables rapid identification of the presence

of this substance in the beverage sample. The results of the analysis are displayed in real-time on an integrated LCD. This display will inform the user of the presence or absence of the substance. The touch-responsive LCD allows the user to interact with the device, enabling them to control various settings, rerun the test, and start and stop the measurements.

The primary application of this Raman spectrometer is in venues such as bars, clubs, and social events, where the risk of drink tampering is a significant concern. This project's development and deployment could have a substantial impact on public health and safety, offering a new tool for the fight against substance abuse.

2.1 Project Motivation

Drug-related incidents in bars and clubs pose a threat to public safety and well-being. Therefore, there is an urgent need for innovative solutions to combat this issue. This project proposes the development of a Raman spectrometer designed for the rapid and accurate detection of GABA in drinks. The designed Raman spectrometer aims to provide a user-friendly, efficient, and reliable method for the public, to ensure the safety of the drinks they consume.

The motivation behind this project stems from a critical and growing concern for public safety in social environments. Drink spiking, a form of substance abuse where individuals unknowingly consume drinks laced with drugs or other illicit substances, has seen a disturbing uptick in recent years. Such actions can lead to severe health consequences, including hospitalization, and in extreme cases, even death. Moreover, the psychological impact on victims and the broader societal implications makes this issue a public safety priority.

Raman spectroscopy offers several advantages over existing detection methods for identifying illicit substances in drinks. One of the most significant benefits of Raman spectroscopy is its non-destructive nature. It does not require the sample to be altered or prepared in any way, meaning the drink can be tested and then consumed as normal if no illicit substances are detected. Also, it can typically provide results in seconds. This quick turnaround is crucial in busy bar and club environments. Raman spectroscopy is also highly sensitive and can detect even trace amounts of substances, as well as identify a wide range of illicit substances that might be used in drink spiking. In contrast to other methods, Raman spectroscopic devices are straightforward to operate, meaning little technical expertise and training is required. Although the initial investment in a Raman spectrometer might be higher than other testing methods, its durability, minimal maintenance costs, and the lack of need for consumables (like test strips or reagents) can make it more cost-effective overtime.

In conclusion, the Raman spectrometer project is driven by the need to improve public safety in bars and clubs, with technology offering a practical, efficient, and

versatile solution to the challenges posed by current substance detection methods.

2.2 Project Goals and Objectives

The basic goals for this project encompass several key aspects. The basic goals of this project are:

- Develop a system capable of accurately determining the presence of GABA (in lieu of GHB) within liquid samples at and above a threshold defined experimentally.
- Enhance spectral resolution to enable finer analysis of molecular structures and compositions, aiming for a spectral resolution of approximately 1nm or better.
- Establish efficient data acquisition and processing methodologies to streamline analytical procedures. This includes:
    - Developing algorithms for efficient acquisition of Raman spectra.
    - Optimizing exposure times and signal-to-noise ratios.
- Create a user-friendly interface to ensure accessibility and ease of operation for researchers of varying expertise levels.
- Focus on cost optimization to deliver high performance at an affordable price point, thus maximizing the instrument's accessibility.
- Incorporate a motorized rotation stage to enable precise measurements.

The objectives to obtain the basic goals are listed below.

- To determine the threshold at which our Raman spectrometer can detect the presence of GABA, the Raman spectrometer will be calibrated using known concentrations in an experimental set up. This will be compared to a baseline spectrum of pure GABA.
- To reach a spectral resolution of 1nm or better, different optical configurations will be tested, and narrow-band filters or advanced dispersive elements will be utilized.
- To develop algorithms for efficient acquisition of Raman spectra, software tools for real-time spectral processing, including background subtraction and baseline correction will be implemented. It will be validated by comparison with known reference spectra.
- A user-friendly interface will be developed by implementing an intuitive touchscreen interface for easy spectrometer control and data visualization. Selectable options for identifying the liquid in which the sample is immersed, and a real-time substance detection output will also be implemented.
- Cost-effective alternatives for optical parts will be evaluated for trade-offs between cost, performance, and reliability.

- To make the rotation stage effective, a code will be developed to move in discrete steps and to automatically home it after the spectrum has been measured.

The advanced goals for the project are outlined as follows:

- Focus on laser power optimization to enhance signal-to-noise ratios and improve sensitivity in detecting molecular vibrations. This involves:
    - Fine-tuning laser parameters such as intensity and duration to achieve optimal performance.
    - Minimizing sample damage during the optimization process.
- Expand the wavelength range of the spectrometer to enable the analysis of a broader range of materials and molecules. This may involve:
    - Incorporating additional laser sources.
    - Modifying existing laser sources to enhance the spectrometer's versatility.
- Develop a sophisticated sample handling system to facilitate:
    - Automated sample positioning.
    - Manipulation and analysis of samples.
    - This system aims to streamline experimental workflows, increase throughput, and ensure reproducibility in data acquisition, advancing the efficiency and effectiveness of Raman spectroscopy applications.

The objectives to obtain the advanced goals are listed below:

- Comprehensive analysis and experimentation to determine the optimal laser parameters, which include:
    - Wavelength
    - Power
    - Pulse duration
    - Development of advanced laser control systems capable of dynamic adjustment.
- Evaluation of available laser sources and optical components to:
    - Cover a broader spectral range.
    - Modify existing components as necessary.
- Design and integration of customized sample holders, stage systems, and robotic handling mechanisms specifically tailored to Raman spectroscopy experiments, involving:
    - Precise control interfaces.
    - Validation testing for reliability and compatibility.

These objectives aim to collectively enhance the performance, versatility, and efficiency of the Raman spectrometer, advancing its capabilities for diverse spectroscopic applications.

The stretch goals for the Raman spectrometer project can be summarized as follows:

- Achieve a compact and portable design to enhance accessibility and enable field-based or on-site analyses.
- Strive for multi-substance capability to expand the spectrometer's applicability by enabling:
    - Simultaneous detection and differentiation of multiple substances within a single sample.
- Target advanced spectral resolution enhancement techniques to further refine the instrument's analytical precision and sensitivity, potentially involving:
    - Fourier-transform Raman spectroscopy.
    - Advanced signal processing algorithms.
- Integrate advanced data processing and machine learning techniques to:
    - Automate analysis workflows.
    - Improve detection accuracy.
    - Enable real-time decision-making capabilities.

These goals aim to elevate the Raman spectrometer's performance and versatility, pushing the boundaries of spectroscopic research and application.

The objectives to meet the stretch goals for the Raman spectrometer are outlined as follows:

- Design a compact and portable system by:
    - Conducting component analysis to identify and utilize lightweight materials.
    - Optimizing housing design to enhance mobility and versatility.
- Enable multi-substance capability through:
    - Refining algorithms for enhanced detection and differentiation.
    - Optimizing laser configurations for broad-spectrum analysis.
    - Implementing multi-channel detection systems for accurate analysis of complex mixtures.
- Explore and integrate advanced spectral resolution enhancement techniques such as:
    - Coherent anti-Stokes Raman scattering (CARS) for fine spectral feature extraction.
    - Optimized signal processing algorithms to enhance detection sensitivity.
- Integrate advanced data processing and machine learning techniques by:
    - Developing software frameworks suitable for spectroscopic analysis.
    - Training machine learning models for improved detection accuracy.
    - Implementing feedback mechanisms to automate analysis workflows and enhance accuracy over time.

These objectives represent a comprehensive approach to realizing the full potential of the Raman spectrometer, aiming to significantly advance its analytical capabilities and application scope.

2.3 Optical Layout of RAID

In this section, we delve into a comprehensive visualization of our optical system using Blender, a robust 3D rendering software. This visualization serves as a crucial tool for understanding and analyzing the intricate configurations and interactions within the optical system. By leveraging Blender's advanced rendering capabilities, we have created detailed models that not only depict the physical layout and components of the system but also simulate the optical behaviors and light path trajectories.

The rendering process involved meticulous attention to detail in modeling each optical component, including lenses, mirrors, and light sources, to ensure accuracy in the depiction of light propagation and interaction. This visualization not only aids in the diagnostic assessment of the system’s efficiency and performance but also provides a visually engaging means to communicate complex optical principles and alignments to a broader audience, including stakeholders and team members who may not have specialized knowledge in optics.

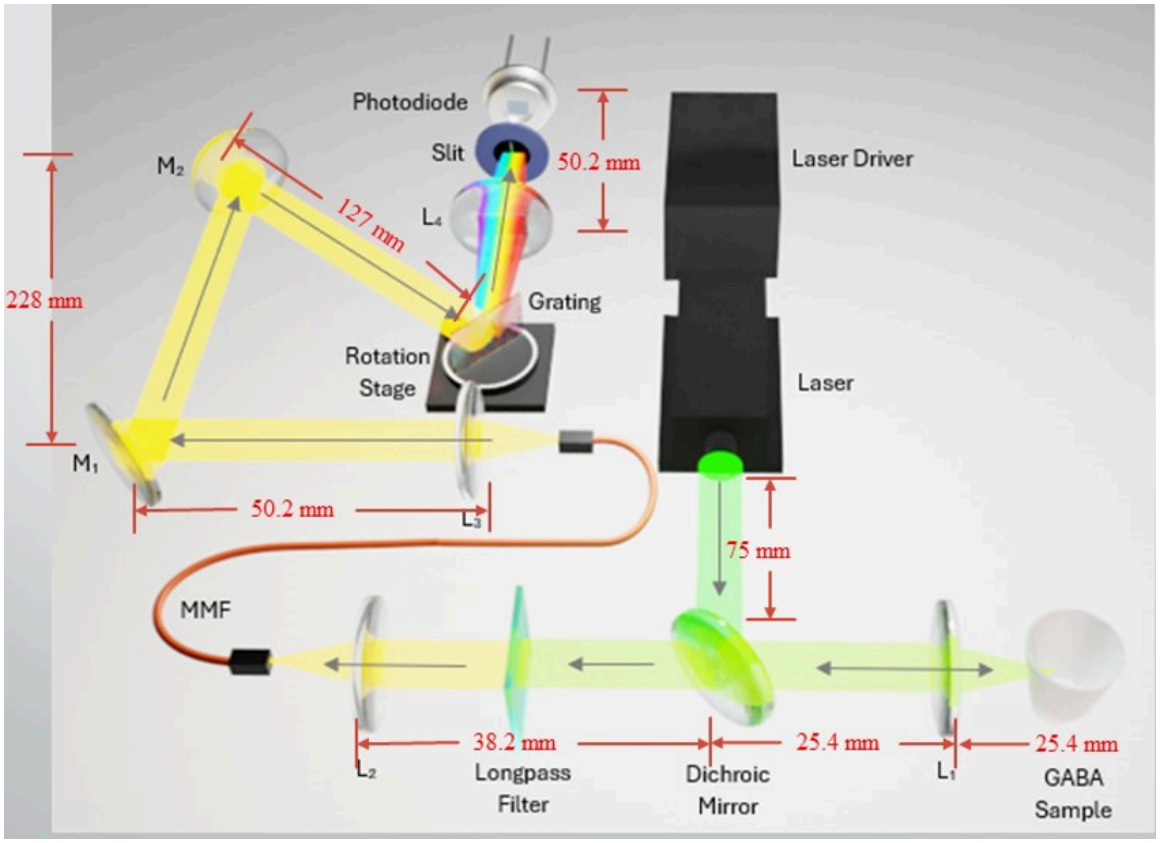


Figure 2.3.1 Optical Schematic

2.4 Project Block Diagram

The RAID project's primary hardware components are depicted in Figure 2.6, where each block is color-coded to indicate the respective team member's responsibility. The system consists of three main subsystems. The first is dedicated to capturing Raman signals and transmitting the received information through an optical fiber. The second subsystem involves the spectrometer, where these transmitted Raman signals are then processed through a CCD. The CCD works with the microcontroller and in-house software to create a detailed analysis of Raman spectra. The third subsystem integrates the analyzed data into a user-friendly interface displayed onto an LCD screen. This project requires extensive system integration, with the spectrometer phase demanding interdisciplinary collaboration to ensure the successful completion and

functionality of the entire project.

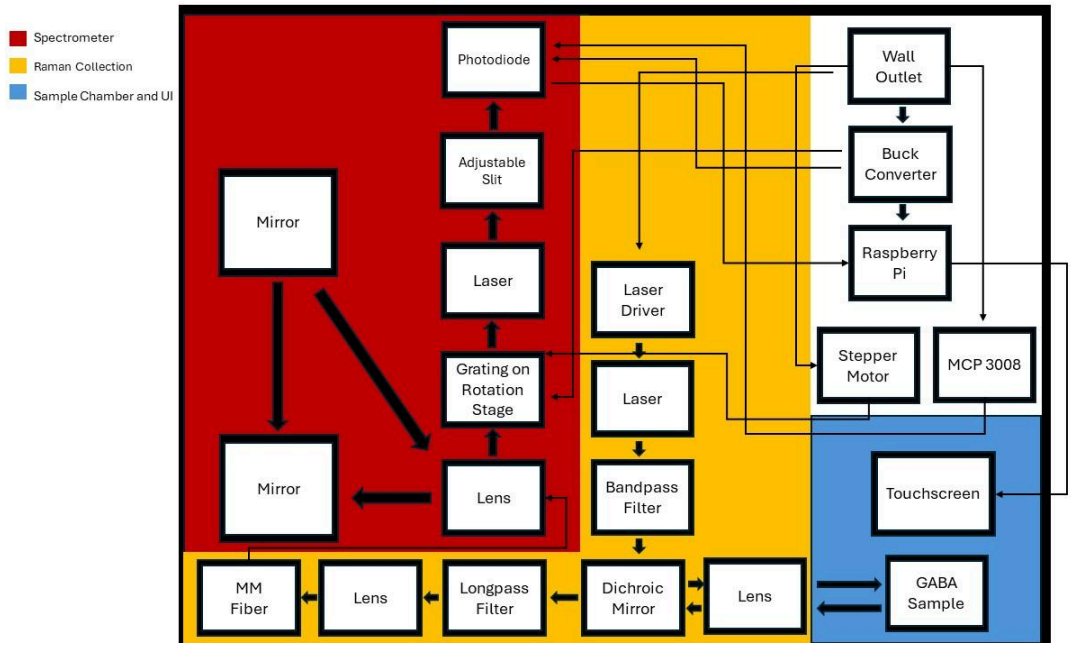


Figure 2.4.1 Hardware Block Diagram

2.5 Project Software Diagram

The implementation of the project necessitates the integration of software for the analysis of data acquired by the photodetectors. As depicted in Figure 2.7, a concise overview outlines the strategy for ascertaining the detection of GABA for the demonstration. The sensor generates data, which is subsequently transmitted to a detection algorithm. This algorithm employs statistical analysis to discern the presence or absence of GABA. Depending on the outcome, whether such substance is detected or not, the result is then relayed to the LCD user interface display.

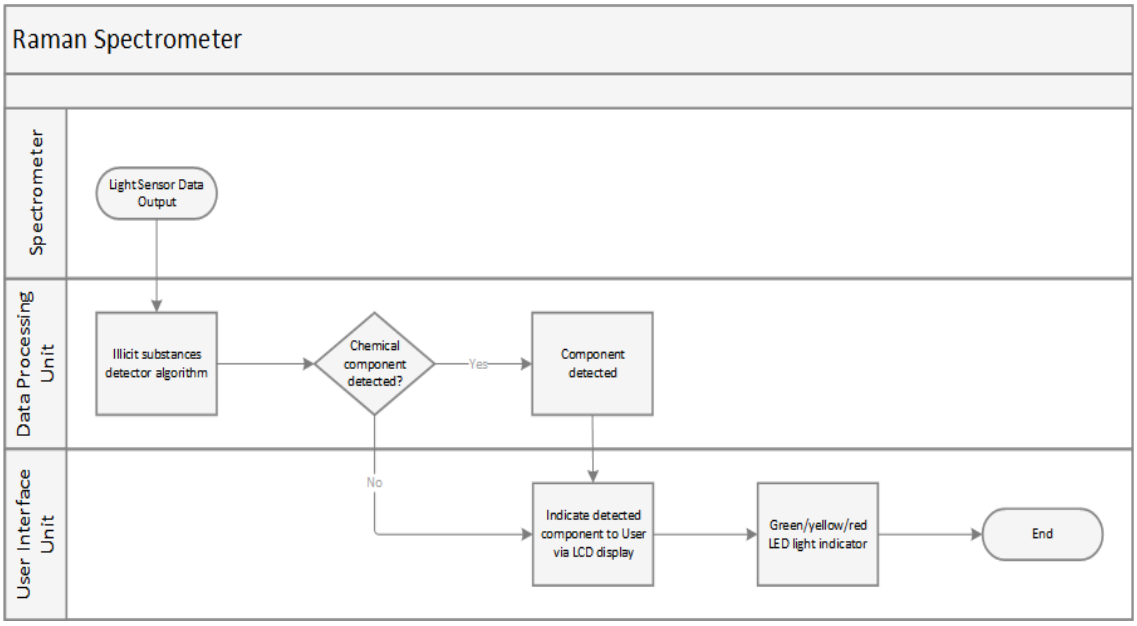


Figure 2.5.1 Software Block Diagram

2.6 House of Quality

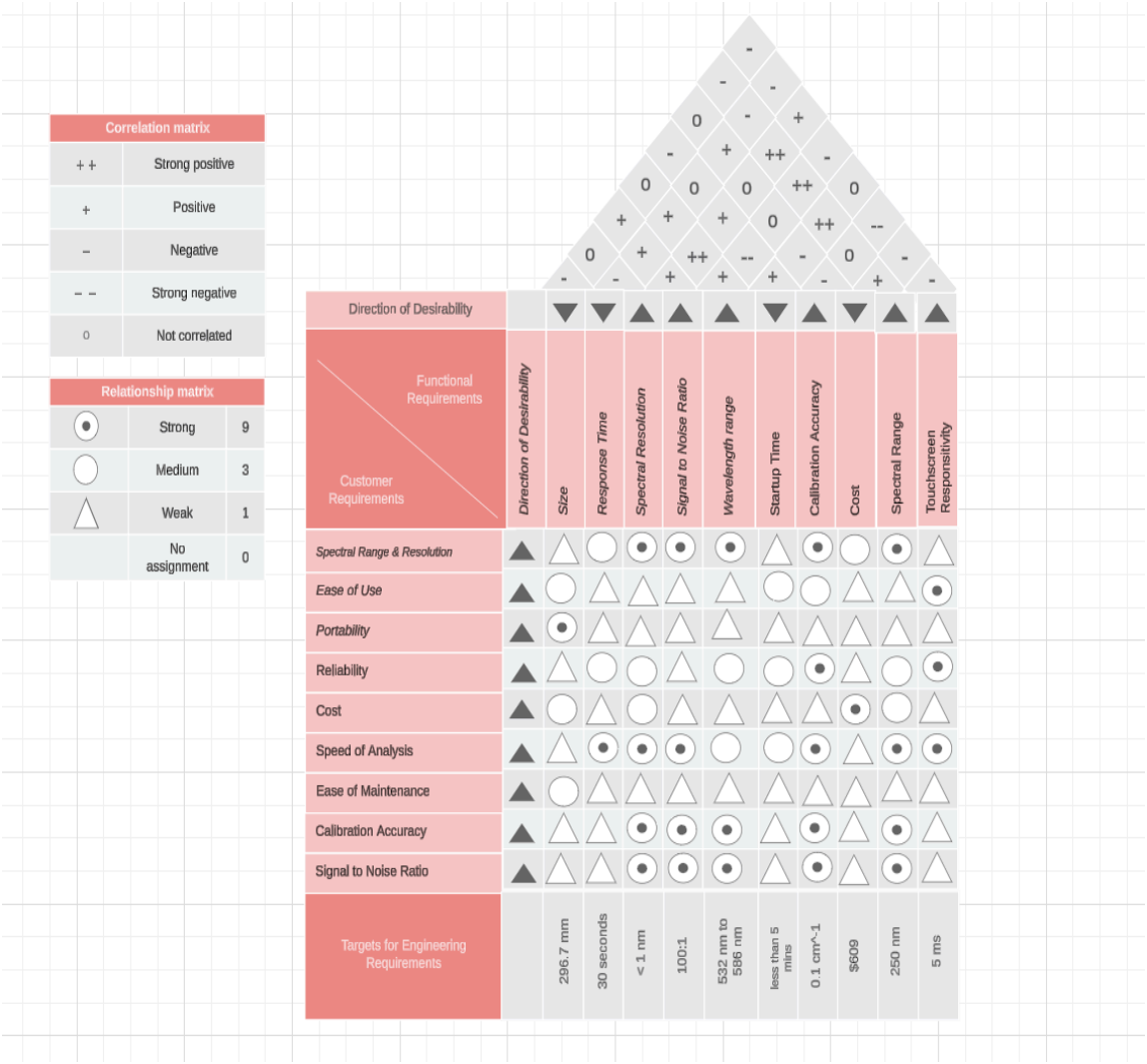


Figure 2.6.1 House of Quality

3 Research and Part Selection

This section will focus on the research conducted into the varying technologies available for implementation in this project. Subsequent specific part selection will be conducted based on the most methodically appropriate chosen technology.

A rigorous investigative process regarding technology selection has a direct correlation to making well-informed product purchasing decisions. Failing to complete a comprehensive and proper investigation covering a variety of relevant and accessible technologies that also house the capability to deliver solutions aligned with our Raman spectrometer requirements, would result in the project being susceptible to errors based on assumptions. The technology investigation will span a substantial array of topics across multiple disciplines. Examples include but are not limited to light sources, rotating stages, and microprocessors.

After completing said research, the specific parts will be selected based on a comparative analysis of diverse components within similar technology. While many of these technologies are multifunctional and could be used in a variety of situations, it is crucial to prioritize our project objectives and primary goals. Concisely, each selected part must meet the criteria for at least two project goals while all the parts combine collectively to meet the overall goals.

Collectively, the parts selected must adhere to all listed objectives to realize our project goals. Selecting a microprocessor that does not have enough memory could result in the algorithm not reading the proper result from the light source and potentially providing a false positive or otherwise deceptive result. Such an occurrence could potentially mislead the user into thinking that their beverages are safe for consumption. Selecting a rotating stage that has a high price point would result in an overpriced Raman Spectrometer which would not align with our cost-effective goal. A glitchy touch screen could make the user experience unpleasant and frustrating. Each part must meet its requisite objectives and assist in fulfilling the goals of the project.

3.1 GABA

3.1.1 Experimental Methodology

Gamma-Aminobutyric Acid (GABA), a key neurotransmitter in the central nervous system, was analyzed using Raman spectroscopy to elucidate its vibrational properties. For this experiment, GABA was prepared in its powdered form and suspended in a suitable liquid solvent within a cuvette to ensure homogeneity and clarity of the spectral data. A 532 nm laser was utilized as the excitation source due to its efficacy in reducing fluorescence interference, thus providing cleaner Raman spectra.

In the paper, Surface-Enhanced Raman Scattering Spectroscopy for the Detection of Glutamate and γ-Aminobutyric Acid in Serum by Partial Least Squares Analysis, by Ali Momenpour T. Monfared et al., the researchers first studied mixtures of glutamate (GLU) and gamma-aminobutyric acid (GABA) in pure water (de-ionized water) using a technique called SERS (Surface-Enhanced Raman Spectroscopy). Their goal was to identify unique spectral fingerprints (peaks) for each molecule. Water was chosen because it's a simple environment with minimal interference, allowing clear peaks from GLU and GABA to be observed.

They created eight different mixtures with varying concentrations of GLU, GABA, and nanoparticles (used for SERS enhancement). By analyzing the SERS spectra, they assigned specific peaks to each molecule. For instance, a peak around 832 cm^-1 was attributed to GLU, while a peak near 858 cm^-1 belonged to GABA. Interestingly, some peaks appeared in both molecules, likely due to shared functional groups.

The analysis revealed a clear trend: the intensity of GLU peaks changed more dramatically than GABA peaks when their concentrations were adjusted. This difference is likely because GLU has an extra carboxylic acid group compared to GABA, leading to more pronounced vibrational modes.

The good correspondence between SERS peaks and molecule concentrations in pure water suggested the possibility of a simple calibration model for detection. However, for even lower concentrations (micromolar range), the researchers planned to use a more advanced technique called Partial Least Squares (PLS) for better accuracy.

This study provides valuable insights into the Raman spectral characteristics of gamma-aminobutyric acid (GABA), laying the groundwork for its detection using conventional Raman spectroscopy techniques. While the research employed Surface-Enhanced Raman Spectroscopy (SERS) for analysis, the identified Raman peak positions for GABA can be directly translated to conventional Raman measurements.

This paper's findings are applicable to regular Raman spectroscopy for GABA determination:

- **Specificity of Raman Peaks:** The study assigned specific Raman peak positions (e.g., 858 cm^-1) to vibrational modes within the GABA molecule. These peak positions are intrinsic properties of GABA and remain consistent regardless of the Raman technique employed (SERS or conventional).
- **Minimal Water Interference:** The researchers utilized de-ionized water as the solvent for their SERS measurements. Water exhibits weak Raman scattering, minimizing its interference with the Raman peaks of GABA. Therefore, the observed GABA peak positions can be reliably transferred

to scenarios using aqueous environments in conventional Raman spectroscopy.

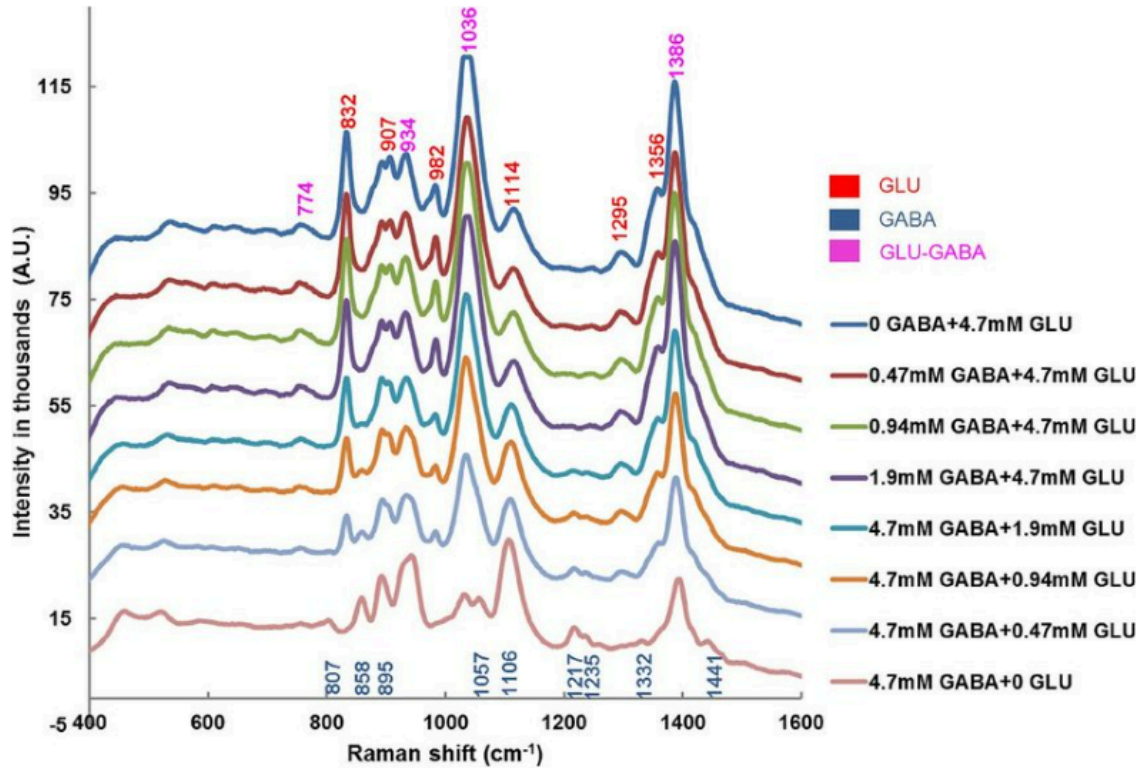
- **Chemical Identity, not Enhancement Mechanism:** SERS enhances Raman scattering through a localized electromagnetic effect near the metal nanoparticles. However, the fundamental information about the molecule's vibrational modes is encoded in the peak positions, not the enhancement mechanism. Consequently, these peak positions can be observed in conventional Raman spectra without the need for SERS enhancement.design

Limitations to Consider:

- **Concentration Dependence:** While the study observed a good correspondence between peak intensities and GABA concentration in pure water, these relationships might require re-evaluation for different solvents or complex biological matrices used in conventional Raman spectroscopy.
- **Baseline Variations:** Conventional Raman spectra can exhibit background signal variations due to solvent or sample matrix effects. Careful baseline correction might be necessary to isolate the characteristic GABA peaks identified in this study.

In conclusion, this paper offers a valuable reference for determining the Raman peaks of GABA using conventional Raman spectroscopy. The identified peak positions for GABA can be directly applied for analysis, although considerations should be made for potential concentration-dependent effects and baseline variations in different measurement environments.

The graph depicted here illustrates the Surface-Enhanced Raman Scattering (SERS) spectra of a glutamate (GLU) and gamma-Aminobutyric acid (GABA) mixture in deionized water, sourced from the study "Surface-Enhanced Raman Scattering Spectroscopy for the Detection of Glutamate and γ-Aminobutyric Acid in Serum by Partial Least Squares Analysis". This visual representation is instrumental for comparing and contrasting the spectral peaks of GABA as identified through SERS with those obtained from other Raman spectrometers. The graph effectively displays various concentrations of GABA in the presence of GLU, highlighting the characteristic peaks that can be used to distinguish between the two compounds. These peaks serve as benchmarks for assessing the performance and accuracy of Raman spectrometry in detecting and measuring GABA in different sample matrices.



SERS spectra of GLU-GABA mixture in DI water.

Figure 3.1.1 Graph displaying the Raman peaks of GABA

3.1.2 Raman Spectral Analysis

The Raman spectrum of GABA was recorded over a range from 300 cm^-1 to 3000 cm^-1. This range includes significant vibrational modes that can be attributed to the molecular structure of GABA, encompassing stretches and bends that are characteristic of its functional groups.

1. Low-Frequency Region (300 cm^-1 - 800 cm^-1): This region typically exhibits skeletal vibrations and lattice modes in molecular crystals. For GABA, prominent peaks were likely observed due to out-of-plane bending modes and torsional vibrations of the molecule.
2. Fingerprint Region (800 cm^-1 - 1800 cm^-1): This crucial region provides the most distinctive features of GABA's Raman spectrum. Key peaks include:
   - Around 850 cm^-1, attributed to the C-C stretching vibrations.
   - Near 1040 cm^-1, possibly representing the C-N stretch vibrations, indicative of the amino group in GABA.
   - A strong band around 1400 cm^-1 could be associated with the COO- symmetric stretching vibration, characteristic of the carboxylic acid group in its deprotonated form.

3. High-Frequency Region (1800 cm^-1 - 3000 cm^-1): This segment of the spectrum highlights the vibrational modes of hydrogen-containing groups:
    - Peaks near 2850 cm^-1 and 2930 cm^-1 are generally attributed to the C-H stretching vibrations of the methylene groups.

The Raman spectrum of GABA obtained using a 532 nm laser source provides significant insight into the molecular vibrations that are characteristic of its structure. The observed spectral features are consistent with the molecular composition and are indicative of the functional groups present within GABA.

3.2 Raman Excitation and Collection

3.2.1 Excitation Setup

Our Raman spectroscopy system features a 532 nm, 500 mW laser, selected for its effectiveness in exciting Raman scattering across a variety of samples. This wavelength minimizes autofluorescence in organic and biological materials while maximizing Raman scattering efficiency, suitable for diverse analytical needs. A function generator modulates this laser, allowing precise control over intensity, pulse duration, and repetition rate. This modulation optimizes the laser-sample interaction, enhancing the Raman signal and reducing potential thermal damage to sensitive samples.

The modulated laser beam is directed towards a dichroic mirror, chosen for its high reflectivity at 532 nm and its ability to transmit longer-wavelength light. The mirror reflects the laser beam, which is then focused by a 25 mm focal length lens onto the sample. This focusing ensures a concentrated laser spot for high spatial resolution and maximizes power density at the sample, crucial for a strong Raman signal from small or heterogeneous samples.

3.2.2 Detection Setup

Post-interaction, the scattered light from the sample is collected and collimated by the same lens used for focusing the excitation light. This lens serves the dual purpose of focusing and collecting light, improving the optical efficiency. The collimated light passes back through the dichroic mirror, which transmits the longer-wavelength Raman-scattered photons while reflecting residual laser light, thereby cleaning the signal.

A long-pass optical filter then further purifies the Raman-scattered light. This filter eliminates any light below a certain wavelength, including stray laser photons, ensuring that only Raman-shifted light reaches the spectrometer. This is vital for reducing background noise and enhancing the signal-to-noise ratio of the Raman spectra.

The spectrometer, which includes a diffraction grating and a detector array designed to disperse and detect light across a spectrum of wavelengths, receives the Raman spectrum via multimode fiber. This setup captures the detailed Raman spectrum, where peaks correspond to the vibrational modes of the molecules within the sample. Analyzing this spectral data reveals chemical compositions, molecular structures, and other important properties of the sample.

This Raman setup—incorporating controlled laser excitation, precise optical filtering, and detailed spectral detection—provides a robust framework for obtaining high-quality spectral data from a wide range of samples.

3.2.3 Types of Raman spectroscopy

Raman spectroscopy has many variants, each with specific applications and advantages, making it crucial to select the most appropriate form of Raman spectroscopy based on the analytical requirements. The following are the different types of Raman spectroscopy:

1. **Spontaneous Raman spectroscopy (SRS)** is the most fundamental form of Raman spectroscopy. It is characterized by its simplicity and direct approach, which involves illuminating a sample with a laser and detecting the scattered light. The key feature of SRS is its ability to provide detailed vibrational spectra, offering insights into the molecular structure of the sample. This is the approach that we have decided to use in our project. We will go further in depth to why this decision was made in the following section.

2. **Resonance Raman spectroscopy (RRS)** enhances the Raman signal for certain resonant molecules, making it highly suitable for studying molecules that can absorb the laser light used. RRS exploits the resonance effect, which occurs when the wavelength of the excitation laser closely matches an electronic transition wavelength of the molecule of interest RRS is particularly advantageous for studying biological pigments due to its ability to provide enhanced signals from specific molecular groups. However, its specificity can also be a limitation, as it is less versatile.

3. **Surface-Enhanced Raman spectroscopy (SERS)** significantly increases the Raman signal by utilizing nanostructured metal surfaces, making it powerful for trace analysis. These metal nanoparticles create localized electromagnetic fields when illuminated by laser light, leading to an enhancement of the Raman signal by many orders of magnitude. This enhancement enables the detection of molecules at very low concentrations. However, the need for specialized substrates and the potential influence of the surface on the sample limit its application scope.

4. **Coherent Anti-Stokes Raman spectroscopy (CARS)** is a nonlinear process offering higher sensitivity and resolution that SRS, which is useful for studying molecular dynamics in real time. It involves two laser beams with different frequencies interacting with the sample. The difference in their frequencies is matches to a vibrational frequency of the molecule of interest. CARS generates a coherent signal, which can be orders of magnitude stronger than spontaneous Raman signals, allowing for the high-resolution imaging of samples and the study of dynamic processes in real time. Its complex setup and the requirement for sophisticated equipment, however, make CARS more suited for specialized applications rather than routine analysis.

Each of the Raman spectroscopy techniques has specific strengths and limitations. The choice among them depends on the requirements of the analysis. The decision to use SRS for GABA detection in liquids is rooted in several critical advantages:

1. Simplicity and Directness: SRS does not require complex sample preparation of the use of enhancing agents, which could interfere with the GABA signal or introduce artifacts.

2. Broad Applicability: Unlike RRS or SERS, SRS does not rely on the presence of specific functional groups or the use of enhancing substrates, making it universally applicable to a wide range of molecules, including GABA.

3. Non-Destructive and Highly Specific: SRS provides a highly specific fingerprint of molecular vibrations, enabling the precise identification of GABA among other substances without altering the sample.

4. Sensitivity to Low Concentrations: Although SRS is generally less sensitive than techniques like SERS or CARS, advancements in detector technology and signal processing have significantly improved its ability to detect low-concentration compounds like GABA in complex biological matrices.

Spontaneous Raman spectroscopy offers a unique combination of simplicity, specificity, and sensitivity, making it an ideal choice for detecting GABA in liquid samples. While SRS presents a promising solution for the detection of drugs in beverages, challenges such as fluorescence interference, the need for database development for spectral interpretation, and the cost of high-resolution instruments remain. Future research directions include the enhancement of signal processing algorithms, integration with artificial intelligence for automated analysis, and the development of more compact and cost-effective spectrometers.

3.2.3.1 Rationale for Wavelength Selection

The selection of the 532 nm wavelength for Raman excitation in our spectroscopic analysis is based on several key considerations that optimize both the efficiency and quality of the Raman scattering process. This wavelength, which corresponds to the second harmonic of an Nd:YAG laser, is prevalent in Raman spectroscopy due to its strong interaction with a wide range of materials and its ability to induce a significant Raman scattering cross-section.

3.2.3.2 Advantages of 532 nm in Raman Spectroscopy

1. High Raman Scattering Efficiency: The efficiency of Raman scattering is inversely proportional to the fourth power of the wavelength of the incident light (λ^(-4) dependency). This means shorter wavelengths, like 532 nm, inherently enhance the Raman scattering effect more than longer wavelengths. The 532 nm laser strikes an optimal balance by providing substantial scattering efficiency while still being practical and relatively safe to handle in laboratory settings.

2. Reduced Fluorescence Background: One of the common challenges in Raman spectroscopy is the fluorescence interference caused by the excitation light. Fluorescence often masks the weaker Raman signals because it is generally much more intense. The 532 nm wavelength is particularly effective in minimizing fluorescence from organic and biological samples compared to UV or shorter visible wavelengths, which can excite more broad and intense fluorescence backgrounds.

3. Compatibility with Optical Components: The green light of the 532 nm laser is well-matched with standard optical components and detectors. Many commercially available optical filters, mirrors, and lenses are optimized for the visible spectrum, including the 532 nm range. This compatibility facilitates a more straightforward and cost-effective setup compared to systems that require specialized components for UV or IR wavelengths.

4. Enhanced Signal-to-Noise Ratio: Using 532 nm allows for a clearer distinction between the Raman signal and the Rayleigh scattered light, which remains at the excitation wavelength. The capability to effectively filter out the intense Rayleigh scattering while capturing the shifted Raman signal is crucial for acquiring high-quality spectral data. The inherent properties of 532 nm light assist in achieving a higher signal-to-noise ratio, crucial for detecting low-concentration components in a sample.

3.2.3.3 Implementation in Our Setup

In our Raman spectroscopy system, the 532 nm laser was precisely modulated and focused to interact efficiently with the sample. The wavelength's enhanced scattering efficiency and reduced fluorescence excitation are vital for our objective of obtaining clear, distinct Raman spectra from diverse materials. By leveraging the specific advantages of the 532 nm wavelength, we ensured that our spectroscopic analyses were both sensitive and selective, providing reliable insights into the molecular structure of the investigated samples.

The selection of a 532 nm laser for the Raman excitation of GABA is a strategic decision that leverages the physical and chemical properties of this wavelength to optimize the spectroscopic analysis. This choice ensured enhanced Raman scattering efficiency, reduced autofluorescence, and better compatibility with standard optical components, culminating in reliable and high-quality spectral data. This allowed for a more precise and detailed analysis of GABA's molecular structure and dynamics, which is invaluable in both research and clinical settings.

3.2.4 Measuring the Laser Beam Diameter

The quality of the Raman signal is heavily influenced by the focusing properties of the laser beam used to excite the sample. Thus, precise control over the beam's spatial characteristics is essential for the effective design and optimization of a Raman spectrometer. This section details the procedure and results of measuring the laser beam size utilizing a beam profiling camera coupled with DataRay software, aiming to determine the focal lengths of all lenses within the spectrometer.

The experiment was conducted using our 532nm laser with the beam directed through a 4.0 OD Neutral Density (ND) filter. A beam profiling camera was placed along the path to capture the spatial profile of the beam. The beam size measurement was conducted using DataRay software. The software enabled the precise measurement of the beam's width at the $1/e^2$ intensity level, which is a standard metric for defining a laser beam size. This measurement was crucial for our calculations, as the beam size directly influences the determination of the lens focal lengths required for the spectrometer. As seen in the figure below, the measured beam size was approximately 1.2mm in diameter.

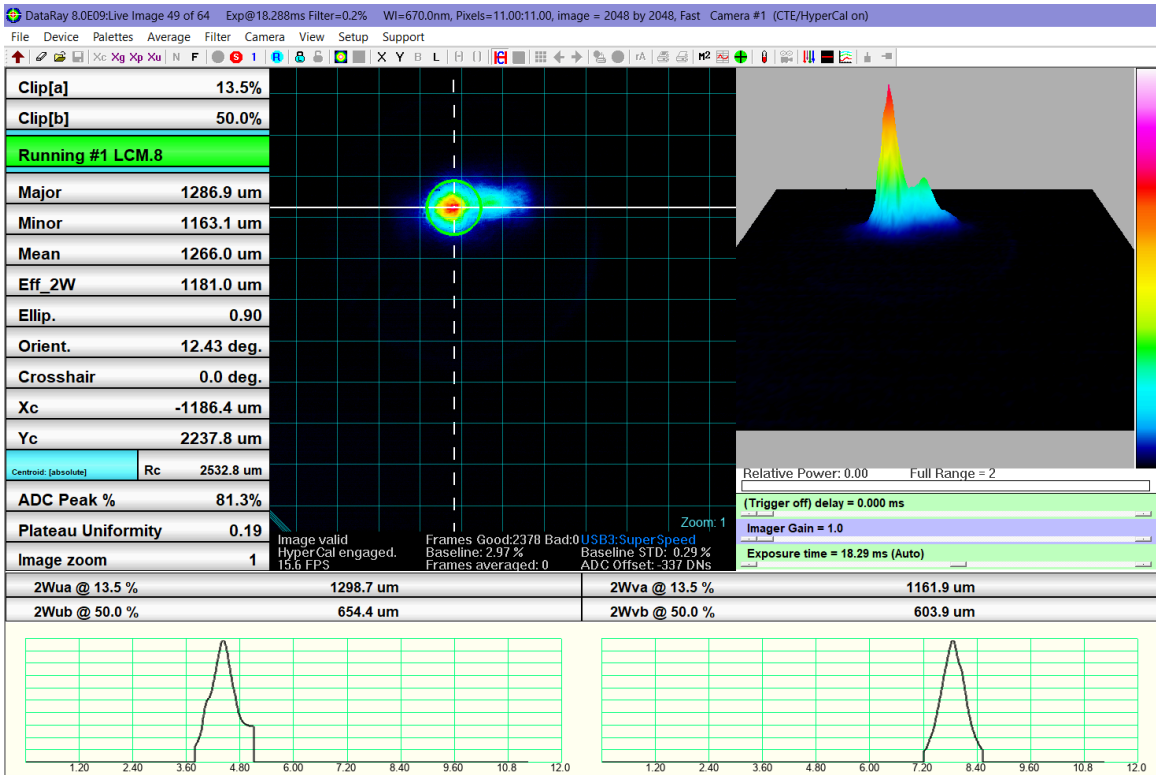


Figure 3.2.1 Laser Beam Diameter using DataRay

The uniformity and quality of the laser beam used as the excitation source are critical factors that influence the technique's sensitivity and resolution. As seen in the figure above, the beam's spatial intensity distribution is irregular, and therefore is not a perfect Gaussian. Traditional perspectives advocate for a laser beam with a Gaussian or similarly regular spatial intensity profile to ensure consistent sample illumination and optimized signal collection. However, under specific circumstances and with appropriate system considerations, the use of a laser beam with an irregular spatial intensity distribution can be acceptable. This section explores the rationale behind the tolerability of employing an irregular beam profile in Raman spectrometry.

An irregular beam profile is acceptable because RAID uses liquid samples. Liquids have a natural ability to scatter light, which can lead to the homogenization of the beam profile as it passes through the sample. This scattering effect can mitigate the irregularities present in the initial beam profile, effectively smoothing out hot spots and other anomalies by the time the light interacts with the molecules of interest. Additionally, the optical setup for liquid-phase Raman spectroscopy can be more forgiving in terms of alignment and focusing requirements. Since the sample itself can partially compensate for beam profile irregularities, there is less need for precise control over the beam's

focus at the sample site, thereby tolerating some degree of spatial intensity variation.

Achieving a clean Gaussian beam profile typically necessitates an optical setup involving multiple lenses for beam shaping and a pinhole for spatial filtering, which collectively “clean” the beam of any irregularities. However, these components add to the bulk, complexity, and cost of the system. Therefore, the acceptance of an irregular beam profile in our design presents a viable strategy for achieving a more compact and cost-effective system.

3.2.5 Manipulation of Laser Intensity

The manipulation of laser intensity is crucial for our setup. This is mainly because we were loaned a 500mW laser, and it is currently assumed that less power is needed to see a Raman signal. Neutral Density (ND) filters, which attenuate laser light through absorption or reflection without altering its spectral characteristics, have been a straightforward solution. Conversely, modulation techniques adjust that power output of the laser source itself, offering a dynamic approach to intensity control. It is important to have meticulous control over laser intensity in Raman spectroscopy to prevent sample damage while ensuring optimal signal strength. This section delves into why modulation of the laser is preferred in the RAID setup.

ND filters, while effective in reducing laser power, offer limited flexibility and can introduce several drawbacks:

- Fixed attenuation levels: ND filters attenuate laser intensity by a fixed amount, limiting the ability to adapt to varying sample sensitivities.
- Optical aberrations: the insertion of another optical element can distort the laser beam, potentially affecting the uniformity and focus of illumination.
- Thermal damage risks: high power lasers can heat ND filters, risking damage to both the filter and the sample.

These limitations underscore the need for a more adaptable and less intrusive method for intensity control in Raman Spectroscopy for drug detection.

Advantages of modulation techniques

Modulation techniques, offer dynamic control of laser intensity through electronic means, presenting several advantages:

1. Enhanced precision and flexibility: electronic control enables instant adjustments to laser power for real-time optimization of the Raman signal.

2. Preservation of beam quality and spectral fidelity: modulation maintains the laser's original spectral properties and beam profile, ensuring the detected Raman signal accurately reflects the molecular structure of the drug compounds.

3. Improved safety and energy efficiency: by effectively pulsing the laser, modulation reduces the risk of sample damage and lowers overall energy consumption, as the laser is not continuously operated at high power.

By offering dynamic, precise, and safe control of laser power, modulation addresses the limitations of ND filters, paving the way for more accurate and reliable drug analysis.

3.2.6 Necessary Components for Excitation and Collection

In our setup, we employ a 532 nm, 500 mW laser as the primary excitation source. This specific wavelength was chosen due to its effectiveness in maximizing Raman scattering while minimizing autofluorescence, making it ideal for a wide range of analytical applications.

To optimize the laser-sample interaction, the output of the laser is modulated using a function generator that adjusts the intensity, pulse duration, and repetition rate. This modulation not only enhances the Raman signal but also mitigates potential thermal damage to sensitive samples. The modulated laser light is then directed toward the sample using a dichroic mirror, which reflects the excitation light while allowing the longer wavelength Raman-scattered light to pass through. This is critical for efficiently separating the excitation light from the Raman signal.

The focused application of the laser light is achieved via a 25 mm focal length lens, which concentrates the laser at the sample site to maximize power density and spatial resolution. This lens also plays a dual role in collimating the scattered light from the sample, enhancing the system's optical efficiency.

Following the interaction with the sample, a long-pass filter is used to further purify the light by blocking any residual excitation light and passing only the Raman-scattered light. The cleaned Raman signal is then directed into a spectrometer, where it is dispersed across a range of wavelengths. The spectrometer's diffraction grating, and detector array capture detailed spectral information, enabling the identification of molecular vibrations that provide insights into the sample's chemical properties.

Our Raman spectroscopy system, through a combination of controlled excitation, precise optical manipulation is designed to provide robust and detailed spectral data.

3.2.7 Optical filter

In the construction of a Raman spectrometer, optical filtering technology is crucial for isolating the Raman scattered signal from other photonic noise, most notably the Rayleigh scattered light. Among the various options for optical filtering, the choice between a notch filter and a longpass filter is significant. This paper section elaborates on the preference of a notch filter over a longpass filter for Raman spectroscopy, along with the considerations that led to the choice of the longpass filter for our design.

The primary advantage of using a notch filter in Raman spectroscopy lies in its high selectivity. Notch filters are designed to block a very narrow range of wavelengths – specifically, the wavelength of the laser light used for excitation, thereby eliminating the Rayleigh scattered light.

Unlike longpass filters, notch filters enable the detection of both Stokes and Anti-Stokes Raman signals. This is because they pass light that is both lower and higher wavelength than the blocked laser line, thus enabling a comprehensive analysis of the sample by capturing a broad range of vibrational modes. A notch filter also usually has a sharper cutoff than a longpass filter, which is critical for capturing Raman signals that occur both close to and far from the laser line. Using a notch filter will enable the analysis of more Raman peaks, which will inherently increase the specificity of the system.

One thing to consider when choosing a filter is the signal-to-noise ratio (SNR). Notch filters are particularly effective in improving the SNR of the Raman spectra. By precisely blocking the intense laser line while passing the Raman scattered light, notch filters significantly reduce background noise. This is especially beneficial for detecting weak signals. While longpass filters can also improve the SNR by blocking Rayleigh scattering, they inadvertently block Raman signals close to the excitation wavelength, potentially losing valuable information.

The decision to incorporate a notch filter instead of a longpass filter in the RAID spectrometer is grounded in the former’s superior selectivity, broader spectral coverage and enhanced SNR. This choice enables our device to determine the presence of GABA in liquids with greater specificity. The use of a notch filter also simplifies the design and operation of the Raman spectrometer. By relying on a single, highly selective filter to eliminate Rayleigh scattering, it is possible to reduce alignment complexities and improve the overall robustness of the system for detecting GABA in liquid samples.

However, despite the benefits offered by notch filters, in this instance, a longpass filter is being employed. The choice is primarily dictated by the integration of a dichroic mirror within the spectroscopy setup, which serves to eliminate the anti-Stokes shifted wavelengths. This choice is necessitated by the system's

existing dichroic mirror, which already effectively eliminates Anti-Stokes shifted wavelengths. Consequently, the longpass filter suffices in this specific context, complementing the mirror's function and simplifying the optical design. It efficiently blocks the undesired shorter wavelengths, including the excitation laser light, while allowing the passage of the longer wavelengths, where the Stokes shifted signals are located. This setup ensures that the essential spectral information is retained for analysis, even though it might not leverage the full advantages of notch filtering in isolating the Raman signals.

3.2.7.1 Longpass Filter Selection

In the development and optimization of Raman spectrometers, the selection of suitable longpass filters is crucial for enhancing instrument performance and measurement accuracy. Longpass filters play a pivotal role in blocking undesired Rayleigh scattered light while transmitting the Raman scattered signal, which is essential for capturing high-quality spectral data. This comparison table presents a concise overview of three popular longpass filters from renowned manufacturers: MKS Newport (20CGA-550), Thorlabs (FELH0550), and Edmund Optics (#47-505). Each filter is evaluated based on critical parameters such as size, cut-on wavelength, transmission wavelength range, thickness, and clear aperture. Such a comparative analysis is invaluable for researchers and engineers in selecting the most appropriate longpass filter for their specific Raman spectrometer configurations, taking into consideration the specific requirements of their applications.

Table 3.2.1 Longpass Filter Comparison

Feature	**MKS Newport 20CGA-550**	**Thorlabs FELH0550**	**Edmund Optics #47-505**
Size	50.8x50.8mm	25.0mm	25.0mm
Cut-on wavelength	550nm	550nm	532
Transmission Wavelength	>570nm	559-2150nm	538.9-1200nm
Thickness	1.1mm	3.5mm	3.5mm
Clear Aperture	≥90% of filter size with film-to-the-edge	Ø21.1 mm	22mm

After careful consideration and a thorough analysis of longpass filters, we have decided to integrate the MKS Newport 20CGA-550 longpass filter into our Raman spectrometer setup. This choice was driven by several compelling factors that make this filter the superior option for my specific application needs. Firstly, the filter's cut-on wavelength of 550 nm aligns perfectly with the spectral range of interest, effectively blocking Rayleigh scattered light while allowing the Raman signa to pass through with minimal attenuation. The filter's exceptional thinness of 1.1 mm minimizes potential optical aberrations and facilitates easier integration into compact optical setups. Moreover, the clear aperture, covering ≥90% of the filter size with film-to-the-edge, ensures maximum usable area with minimal light loss, enhancing the overall sensitivity and signal-to-noise ratio of the spectrometer. These features collectively render the MKS Newport 20CGA-550 longpass filter the optimal choice for achieving high precision and reliability in Raman spectroscopy measurements. We thank MKS Newport for sponsoring this component.

3.2.8 Beam Splitting Mechanism

Another pivotal decision in the context of choosing optical components to enhance the system's performance, sensitivity and specificity is the selection of the beam splitting mechanism. It is common for a traditional 50/50 beam splitter to be used; however, a dichroic mirror often presents significant advantages over a 50/50 beam splitter. This section outlines the rationale behind favoring a dichroic mirror for application in the RAID spectrometer.

The primary advantage of a dichroic mirror lies in its ability to selectively reflect and transmit light based on wavelength, unlike a 50/50 beam splitter that divides incoming light indiscriminately. The dichroic mirror can be designed to efficiently transmit the intense laser light towards the sample while reflecting the Stokes-shifted Raman scattered light with minimal loss. This selective separation maximizes the spectrometer's selectivity by ensuring that a higher proportion of the Raman signal reaches the detector, compared to the equal distribution of light by a 50/50 beam splitter, which invariably leads to a significant loss of the useful signal.

Another advantage of the dichroic mirror is its ability to transmit only 532nm incoming light to the sample and reflect all other wavelengths that may be present in the pump. This inherently enables the elimination of a bandpass filter between the laser and the sample. A dichroic mirror also contributes to a higher SNR in Raman spectroscopy. By transmitting the laser light more efficiently towards the sample and reflecting the Raman scattered light with high efficiency, the dichroic mirror reduces the amount of light that inadvertently reaches the detector. This reduction in background light directly translates to a lower noise level in the detected signal. Furthermore, the ability to minimize the detection of Rayleigh scattered light further improves the SNR, making it easier to distinguish and analyze the weak Raman signals.

Dichroic mirrors offer superior flexibility and customization to match the specific requirements of a Raman spectrometer. They can be engineered to have sharp cutoffs and high transmission or reflection efficiency at specific wavelengths, tailored to the excitation source and the Raman signals of interest. This customization ensures optimal performance by maximizing the collection of relevant Raman signals and minimizing unwanted light.

Compared to a 50/50 beam splitter, a dichroic mirror typically exhibits better thermal stability. This stability is crucial in Raman spectroscopy, where precise wavelength separation and maintenance of optical alignment are essential for accurate measurements. Dichroic mirrors, by virtue of their construction and materials, are less susceptible to thermal expansion, ensuring consistent performance over a wide range of temperatures and operational conditions.

In conclusion, the selection of optical components, particularly the beam splitting mechanism, is pivotal in enhancing the performance, sensitivity, and specificity of a Raman spectrometer like the RAID spectrometer. While traditional 50/50 beam splitters have been commonly used, the advantages presented by dichroic mirrors make them a preferred choice. Overall, the adoption of dichroic mirrors in the RAID spectrometer offers significant advantages in terms of performance, flexibility, and stability, ultimately leading to more accurate and reliable Raman spectroscopy measurements.

3.2.8.1 Dichroic Mirror Selection

Selecting the right dichroic mirror is a critical step in the design and optimization of a Raman spectrometer, as it directly impacts the system's efficiency in distinguishing between scattered and incident light. Dichroic mirrors are specialized optical components designed to reflect certain wavelengths of light while transmitting others, making them essential for directing the light path within Raman spectroscopy systems. This comparative table provides a detailed overview of three notable dichroic mirrors from leading suppliers: MKS Newport (DCM13), Thorlabs (DMLP550T), and Edmund Optics (#86-386). The comparison focuses on key features such as diameter, cut-on wavelength, transmittance range, reflectance band, angle incidence, thickness, and clear aperture. These parameters are crucial for determining the suitability of each mirror for specific Raman spectroscopy applications, ensuring the selected mirror maximizes the system's performance by efficiently separating Raman scattered light from the laser excitation source.

Table 3.2.2 Dichroic Mirror Comparison

Feature	MKS Newport DCM13	Thorlabs DMLP550T	Edmund Optics #86-386
Diameter	25.0mm	0.5in	12.55mm
Cut-on wavelength	552nm	550nm	552nm
Transmittance Range	561.4-790.0nm	565-800nm	561.4-790
Reflectance Band	514.5-543.5nm	380-535nm	514.5-543.5
Angle of Incidence	45	45	45
Thickness	3.5mm	3.2mm	3.5mm
Clear Aperture	22.0mm	> ø11.43mm	8.8mm

Among the evaluated options, the MKS Newport DCM13 dichroic mirror stands out as the best choice for my Raman spectrometer setup, for several compelling reasons. Its 25.0 mm diameter provides a suitable balance between size and optical performance, allowing for optimal integration into the spectrometer design without compromising on light collection efficiency. The cut-on wavelength of 552 nm and the specified transmittance range of 561.4-790.0 nm align closely with the spectral characteristics required for my Raman applications, ensuring that the mirror effectively transmits Raman scattered light while efficiently reflecting the laser excitation wavelength. This precise wavelength separation is crucial for enhancing the signal-to-noise ratio and overall sensitivity of the spectrometer. Additionally, the MKS Newport DCM13's specified angle of incidence (45 degrees) and thickness (3.5 mm) are perfectly suited for the optical geometry of my system, facilitating easy integration and optimal alignment. The clear aperture of 22.0 mm further ensures that a significant portion of the incident light is utilized, minimizing losses and maximizing the effective signal collection. Given these specifications, the MKS Newport DCM13 dichroic mirror emerges as the superior option, offering the best combination of performance, integration compatibility, and optical efficiency for my Raman spectroscopy requirements. We thank MKS Newport for sponsoring this part.

3.2.9 Orientation of Dichroic Mirror

Dichroic mirrors are commonly placed at a 45-degree angle in optical systems for a few practical reasons related to their unique function and the physics of light. Dichroic mirrors are specialized mirrors designed to reflect certain wavelengths

of light while transmitting others. This makes them incredibly useful in applications requiring selective wavelength management, such as in fluorescence microscopy, projectors, and laser optics. Here's why the 45-degree orientation is significant:

1. Maximized Efficiency in Reflection and Transmission: When a dichroic mirror is positioned at 45 degrees to the incident light, it optimizes the efficiency of both reflection and transmission of light based on the coating and the design of the mirror. This angle helps in achieving the desired separation of wavelengths efficiently, directing reflected light and transmitted light into different paths that are easy to manipulate and utilize in optical systems.

2. Convenient Geometry for Optical Pathways: Placing the mirror at a 45-degree angle simplifies the geometry of the optical path. For example, in many optical instruments, this arrangement allows one beam path to be redirected by 90 degrees while another passes straight through. This is particularly useful in devices where space is limited or where beam paths must be compactly arranged.

3. Polarization Effects: At a 45-degree angle, the polarization properties of the dichroic mirror can be fully utilized. Dichroic mirrors are often designed to reflect light of one polarization while transmitting light with the opposite polarization. This angle helps in aligning the polarization characteristics of the mirror with the polarization states of the incoming light, ensuring that the mirror operates as intended.

4. Ease of Integration into Optical Systems: The 45-degree angle is mechanically straightforward to implement and integrates well into many optical designs. It allows for a straightforward setup where components can be mounted in standard configurations, facilitating easier design and assembly of optical systems.

Overall, the choice of a 45-degree angle for dichroic mirrors is driven by the need to effectively manage different wavelengths of light while maintaining a practical and efficient optical system design.

3.2.10 Rationale for box design

Handheld Raman spectrometers have emerged as a potential solution for on-site detection of drugs. However, this section argues that a bar-top-mounted, box shaped Raman spectrometer offers significant advantages over handheld devices for drug detection in bars and clubs. We discuss the limitations of handheld spectrometers in these environments and present the benefits if a bar-top design.

Limitations of Handheld Raman Spectrometers for Roofie Detection in Bars and Clubs

Handheld Raman spectrometers have been explored for on-site roofie detection due to their portability and ability to identify molecular fingerprints of various substances. However, their implementation in bars and clubs faces challenges:

- User proficiency: operating a handheld Raman spectrometer requires a certain level of training and expertise for accurate sample analysis. In a fast-paced bar environment, staff may not have the time or training to conduct proper measurements, potentially leading to inaccurate readings.

- Sample presentation: handheld devices necessitate direct contact with the drink, which can be unhygienic and disruptive to the customer's experience. Spills or contamination from previous samples could also compromise the integrity of subsequent tests.

- Environmental challenges: the bright lights and crowded conditions typical of bars and clubs can interfere with Raman spectroscopy measurements. Handheld devices may struggle to produce reliable results under such conditions.

Advantages of a Bar-top Raman Spectrometer Design

A bar-top Raman spectrometer, designed as a fixed box mounted on the bar, can address the limitations above and has these advantages:

- Ease of use: the bar-top design can incorporate automated sample introduction mechanisms, eliminating the need for staff expertise in operating the spectrometer. Customers can simply place their drink within a designated slot on the bar-top unit for analysis.

- Improved Hygiene: the bar-top design involves a closed sample compartment, minimizing the risk of contamination between tests and ensuring a more hygienic experience for customers.

- Environmental resilience: the bar-top unit can be enclosed in a housing designed to mitigate the effects of ambient light and background noise, leading to more consistent and reliable measurements.

While handheld Raman spectrometers offer on-site roofie detection, a bar-top design presents significant advantages in terms of ease of use, hygiene and environmental resilience. This approach has the potential to improve the accessibility and effectiveness of roofie detection in bars and clubs, contributing to a safer entertainment experience. Further research is needed to optimize the design and performance of bar-top Raman spectrometers. Studies investigating

integration with existing bar infrastructure and customer acceptance of this technology are also warranted.

3.2.11 Housing for System

This section explores the design and implementation of a Raman spectrometer specifically enclosed for the detection of contaminants such as gamma-hydroxybutyrate (GHB) and gamma-aminobutyric acid (GABA) in beverages at social venues like bars and clubs. The objective is to provide a secure, user-friendly device that patrons can use to ensure their drinks are safe from these specific types of drugs commonly referred to as "roofies". The study delves into the enclosure of the spectrometer's excitation and collection systems, the overall housing of the device, and a specialized containment box for the beverages during testing.


RAID
RAMAN ANALYZER FOR ILLICIT DRUGS

Figure 3.2.2 RAID Housing

3.2.12 Enclosure of the Excitation and Collection Systems

The Raman spectrometer's excitation and collection systems are critical components that require protection from environmental interference and damage. Enclosing these components in a dedicated, controlled box within the spectrometer prevents external light sources, dust, and moisture from affecting the accuracy and efficiency of the measurements. This enclosure also safeguards the optical components and sensitive electronics from rough handling that might occur in a high-traffic environment like a bar.

3.2.13 Complete Spectrometer Enclosure

The entire spectrometer is enclosed in a robust, tamper-proof box. This outer enclosure is designed to be durable and secure, resistant to accidental impacts, and attempts at unauthorized access or vandalism. Additionally, the design considers aesthetic and ergonomic factors to ensure that the device blends seamlessly into the bar or club environment while being accessible and straightforward to use for patrons.

3.2.14 Beverage Insertion Box

A key feature of the design is a specialized compartment where patrons can place their drinks. This compartment is equipped with a door that patrons can close securely. Once the drink is inside and the door is closed, the spectrometer automatically begins the scanning process. The compartment is designed to accommodate various sizes of drink containers, from standard glasses to larger cups, ensuring versatility in use.

3.2.15 User Interaction

The interface is user-friendly, requiring minimal interaction. Instructions are provided via simple visual cues on a touchscreen panel integrated into the device, guiding the user through the detection process step by step.

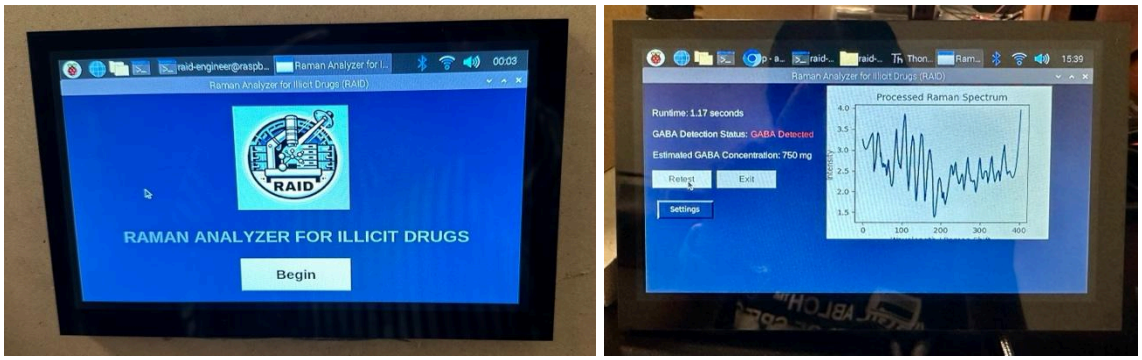


Figure 3.2.3 RAID graphical user interface system

3.2.16 Privacy and Security

The design ensures that all interactions with the device are confidential, with no data stored or recorded to protect patrons' privacy. The enclosure's robust design prevents tampering, ensuring that the integrity of the tests and the device itself are maintained.

The enclosed Raman spectrometer designed for detecting contaminants in beverages at social venues provides a significant advancement in public health safety at bars and clubs. Its robust, user-friendly, and secure design ensures reliable operation and accessibility, making it an invaluable tool for preventing drug-facilitated crimes in social settings.

3.3 Spectrometer Optical Design

Spectrometers have undergone significant technological advancements in recent years which has resulted in improvements in their capabilities and extensions in their applications. One application of spectrometry is using it to characterize materials and analyze chemicals while conducting research in pharmaceuticals. This process takes advantage of the Raman scattering phenomenon, where light interacts with a material through molecular vibrations to produce a unique ‘Raman shift’ characterized by a change in wavelengths. The minimization in handling of illicit drugs is an advantage in Raman spectroscopy which helps in achieving one of the goals of our project, which would see our technology applied in a club or bar like setting.

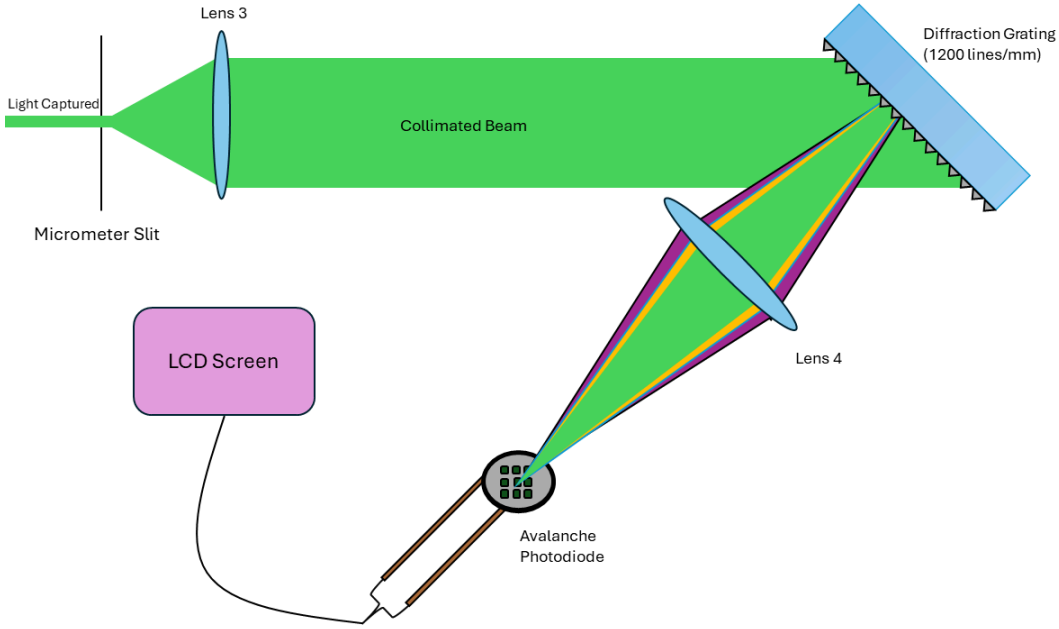


Figure 3.3.1 Spectrometer Optical Setup

Designing and building our own spectrometer gives us control over functionality of the device, which enables us to tailor it to meet certain requirements and specifications. In particular, we determined components of the spectrometer based on measuring the Raman shift of GABA. This neurotransmitter which is a precursor to the illicit drug GHB served as its substitute. Moreover, it enables us to integrate advanced signal processing algorithms tailored to the analysis of GABA's Raman spectra. This device gave us precise identification and concentration of GABA, even in complex sample solutions that are commonly encountered in real-world club/bar like environments.

In addition, building our own spectrometer enables us to not only control its functionality, but we can also take advantage of scaling up the spectrometer and adapting to larger goals if given ample time. By adjusting the spectrometer's parameters such as the slit width, integration time, alignment, and sensitivity, we can potentially detect different compounds. However, it is worth comparing our spectrometer to others available in the market.

3.3.1 Market Comparisons

The first spectrometer we investigated was BRAVO: Bruker's Advanced Handheld Raman Spectrometer. The spectrometer uses a patented method known as Sequentially Shifted Excitation (SSE) Raman spectroscopy. This method uses a distributed Bragg reflector (DBR) laser diode to excite the sample that is necessary to measure. The laser's temperature can be adjusted to achieve precise changes in wavelength, facilitating the accurate application of the SSE

algorithm. SSE produces Raman spectra directly in the true spectral space by sequentially generating multiple excitation spectra with minor variations in wavelength shifts. This leads to improved signal quality compared to conventional methods because it avoids fluorescence interference – which typically distorts the signal.

The BRAVO also has a 2-laser system (785 nm and 852 nm) which provides the user with a large spectral range (3200 – 300 cm^{-1}). This enables adaptability and the measure of multiple substances. Moreover, the system is handheld which is beneficial for achieving our goal of portability. It also uses software that refers to the TicTac Raman Drug Library, which is a database with Raman spectra curated for identifying compounds using Raman spectroscopy.

Being able to take advantage of its portability and detectability and use this device in a club or bar setting would be convenient, but the device requires users to be trained (up to 4 hours) in order to know how to properly use it. The BRAVO's price tag of approximately $60,000 exceeds our budget constraints. It is worth mentioning that deploying such an expensive unit in a club or bar environment would not be practical unless employees are dedicated to monitoring its use (which for $60,000 is not convenient).

Another spectrometer that we investigated was the WP 785X Raman Spectrometer Series. This product contains 3 different systems – fully modular, semi-integrated, and fully integrated systems. This enables users to choose which one is necessary depending on the application of their measurements. The differences between them are their price points and components. The fully modular system uses a laser, Raman probe, sampling optics, and spectrometer separately all connected by fibers while the semi-integrated system combines the spectrometer and laser into one subsystem (with the Raman probe and sampling optics connected separately) for cost effectiveness. The fully integrated system combines the laser, spectrometer, and the sampling optics in one unit, which eliminates the fibers from the system entirely.

The WP 785X series further enhances user flexibility by providing various slit size options tailored to the sample being measured. This feature allows for precise customization, enabling users to optimize their measurements for different samples and experimental requirements. These spectrometers use conventional Raman spectroscopy techniques similar to what RAID uses. Moreover, the system is compact, with the largest one of the series (fully modular system) acting as a moveable station for users. This mobility feature closely aligns with the functionality of our spectrometer in RAID, offering users the convenience of easy relocation and setup.

While the WP 785X series aligns closely with our objectives, its limitation in working distance (from the face of the lens) at 22 mm (about 0.87 in) creates a practical challenge for our intended application in a club or bar setting. In such

environments, where efficiency and ease of use are significant, requiring customers to align their drink samples with the spectrometer would not be feasible. A subscription to their Raman spectra database is also required to properly analyze the sample. Additionally, the software necessitates training, contributing to a lack of user-friendliness for bar customers. Lastly, the spectrometer itself costs roughly $6,000. This does not include the fiber, probe, laser, or other sampling optical components. The WP 785X series unfortunately does not fit our budget.

The final spectrometer we examined was the Pendar X10. This spectrometer uses a technique called Raman Difference Spectroscopy (RDS) which measures a test sample and its reference simultaneously or quickly after each other to obtain a highly resolved spectrum comparison. By subtracting spectra from one another, RDS efficiently removes comparable background signals and highlights the distinctions between them. By highlighting new peaks and peak shifts in the difference spectrum, this method offers in-depth understanding of the structural alterations and differences between the substances under observation.

The Pendar X10 uses a Class 3R laser, there is no requirement for laser safety precautions, which lowers the possibility of ignition. This is especially crucial because the instrument measures substances like chemicals, narcotics, and explosives. The wavelength shift between the two observations has no effect on the fluorescent or ambient light spectra, but it causes a shift in the Raman spectrum equal to the frequency difference between the two Raman lasers. This makes it possible to separate the information-rich Raman component from other signals, making it easier to identify compounds that are colored, mixed, or deteriorated. The software used to analyze the compounds derived from a large library.

Moreover, the Pendar X10's handheld design improves portability, which is essential for accomplishing the goals of our project. Furthermore, the device provides an adjustable standoff distance, which may be adjusted from 1 to 6 feet, thus effectively avoiding contamination from the material or sample being measured. These benefits do not come without a price, though, since the device costs $65,000. In addition, the embedded software requires user training in order to be properly utilized, indicating a less-than-ideal user-friendly experience and placing further financial strain on our project.

The table below lists the precise feature comparisons between these similar devices and the suggested RAID specifications. RAID appears to be a similar, but more cost-effective, device based on its features and specifications sheet, offering most of the characteristics of the top competing devices along with a host of new functions. Similarly, its design covers most of the typical offerings on the market, the most prominent being a user-friendly touch screen for functionality. While these objectives are ambitious, we are confident in our ability to incorporate them into the final design.

Table 3.3.1 Spectrometer Comparisons

Feature	RAID	BRAVO	WP 785X	Pendar X10
Cost	$1,500	$60,000	$7,000	$65,000
Portability	Moveable Station	Portability	Moveable Station	Portability
Training	10 seconds	4 hours	6 hours	<1 day
Operational Duration	> 8 hours	5 hours battery life	> 8 hours	3 hours battery life
Startup Time	< 30 secs	< 45 secs	< 2 minutes	< 1 minute
Measure Multiple Substances	GABA	Yes, TicTac Raman Drug Library	Yes, no public information as to specifics	Yes, explosives, illicit drugs, CWAs, toxic industrial chemicals
Resolution	1E-7	10 – 12	7 – 8	10

In summary, designing and building our own spectrometer not only granted us control over its functionality but also enables us to focus on detecting specific compounds like GABA with high precision and reliability. This tailored approach enhanced the effectiveness of our detection system and strengthened its applicability in various practical settings, including the detection of GABA in club or bar environments.

The optical design for the spectrometer of the RAID project encompasses several essential components, each serving a critical role in the precise and effective identification of substances within beverages (in particular GABA). While deciding on which components are necessary to read and analyze the Raman shift signal, we also consider the labor hours and costs associated with the designs.

When designing the spectrometer, guiding as much light into the system as possible is important and ensuring that the signal is optimized for detection. Initially in this selection process, we thought about using a single-mode fiber to

connect the illumination system to the spectrometer. The benefit of using a single-mode fiber would be that we would have less dispersion that occurs within the fiber. This would ensure that different wavelengths of the light arrive at the end of the fiber simultaneously, thus creating a strong wavefront and preserving the coherence of the signal.

The issue with using a single-mode fiber is coupling the incoming light into it efficiently. Due to these fibers having a core size of a few microns, it causes the process of coupling the signal to be a labor-intensive process requiring more opto-mechanical components to be incorporated (driving up the cost). Considering that our goal is to the Raman Analyzer for Illicit Drugs to be in a bar or club setting, there is a likelihood that the system may be bumped causing misalignment causing signal loss or distortion.

A multi-mode fiber has also been considered because it would enable us to gain spatial coherence when the light propagates throughout the spectrometer's optical system. This spatial coherence would help preserve and maintain the strength of the incoming Raman signal. The multi-mode fiber is easier to couple than the single-mode fiber due to the increase in light propagation paths (modes) that are in the core of the fiber. The addition of these modes would create another problem, as more modes will cause more dispersion to occur.

Any lack of spatial coherence in the instance of RAID's spectrometer may hinder the device's sensitivity and dependability in detecting drugs in beverages in an environment like a club or bar where quick and precise detection is essential. Introducing modal dispersion will cause different modes of light to propagate at different velocities. These wavelengths would arrive at the slit at different times, which might deteriorate the entering light's spatial coherence and cause the spectral characteristics to smear or blur. Lastly, the cost of implementing a multi-mode fiber would be the same as using a single-mode fiber.
Therefore, rather than using fiber to connect the illumination system and the spectrometer we instead decided to use a lens to focus the light onto the slit. The spectrometer can benefit from many advantages when light is focused onto a slit using a lens rather than fiber. To maximize the amount of light that enters the system (used for analysis), it is effective in coupling light into the spectrometer system. By ensuring a higher signal at the detector, this raises the spectrometer's sensitivity and improves the signal-to-noise ratio. Alignment of the lens is dependent on the focal length of the lens in the illumination system. The only downside to using a lens rather than a fiber is the lack of flexibility in positioning of the optical components within the design.

3.3.2 Spatial Filters

When selecting the first component the light interacts with in the spectrometer, we must consider having a spatial filter. Its primary function is to regulate the incoming light beam's size and shape to ensure that we measure the proper

spectral information for the spectroscopic analysis. For GABA, we must account for the central wavelength of 586 nm. Moreover, having a spatial filter reduces the spatial and spectral distortions which are caused by ambient light and aberrations from the lens. This reduction therefore enables sharper spectral peaks to be analyzed by the photodiode. It also improves our signal-to-noise ratio due to the dampening of the noise. This can be better understood by looking at its formula:

$$SNR = \frac{P_{signal}}{P_{noise}}$$

Equation 3.3.1 Signal-to-Noise Ratio formula

The potential reflections that may occur within our illumination optical system would be blocked entirely with the spatial filter. In addition, this removal of unwanted light rays improves the sensitivity and accuracy of the photodiode (detector of spectrometer). This sensitivity refers to the spectrometer's ability to detect and measure the small changes and low concentrations of the molecules within the sample. We have the entire RAID system (illumination system and spectrometer) mostly enclosed with a space for the sample drink to be placed in the path.

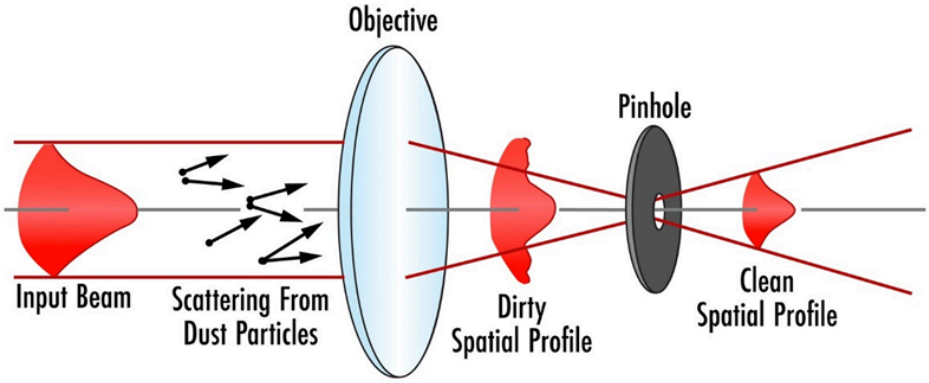


Figure 3.3.2 Pinhole Spatially Cleaning Beam Profile (Edmund Optics – Pending Approval)

Additionally, the light beam can be somewhat collimated via spatial filters to make it more parallel before it hits the grating. However, it cannot entirely collimate the beam and rather assists in the process.

Spatial filters also play a significant role in determining the resolution of the system. Spatial resolution is the detector's ability to discriminate between spectral characteristics that are closely spaced. By adjusting the spatial characteristics of the light beam before its interaction with the spectrometer's optical components,

we can control the spatial information that is captured. Also, the spectral resolution is determined too, which is the detector's ability to resolve spectral lines/features based on a given set of wavelengths. These spectral peaks can typically be expressed as the full width at half maximum (FWHM), which is the peak's width at half of the maximum intensity ($\frac{I_{max}}{2}$).

One variation of spatial filters are pinholes, which are a small aperture (hole) with an adjustable radius controlled by a dial. They can be used as the spatial filter for the spectrometer, offering all the benefits of the spatial filters listed earlier and the benefit of conducting a confocal operation. A confocal operation is a technique used in Raman microscopy, which enables a specific light plane to pass while all other light planes are rejected. This grants us the ability to reconstruct three-dimensional models of the sample we measure by scanning through multiple focal planes. For the project's goals, this is not necessary because our end goal is to determine if the drink is spiked and if so at what concentration.

Another variation of spatial filters is slits, which is a narrow aperture (gap) that can be made adjustable using a knob. Slits provide better control over the light beam's intensity by adjusting height and width. This versatility enables us to better control the amount of light passing through. This adjustment is essential, particularly in applications where sensitivity is critical, for attaining the ideal signal-to-noise ratio and preventing the detector from being overexposed (causing damage).

Moreover, slits make it possible to control how light is distributed spatially. This makes it possible to choose areas of the incoming beam. This feature is especially useful in Raman spectrometry setups where obtaining high-resolution spectra requires spatial coherence and homogeneous illumination. Slits can efficiently sculpt the light beam to fit the needs of later optical elements, such gratings and collimating lenses, providing optimal performance all throughout the system.

When comparing the slit and the pinhole, several distinctions emerge. One of these distinctions is that pinholes often demonstrate lower light throughput compared to slits. Pinholes' intrinsic ability to limit light transmission to a single, small aperture is responsible for this decrease in light transmission. Pinholes usually have set diameters specified by their physical dimensions, unlike slits, which allow changeable widths to control the quantity of light flowing through.

As a result, only a limited portion of the incident light beam can traverse through the pinhole, leading to decreased light throughput. While pinholes effectively eliminate unwanted spatial and spectral components of light, their lower light transmission can impact the overall signal strength in optical systems, necessitating careful consideration of their usage in applications where maximizing light throughput is critical for optimal performance. Although pinholes are an efficient way to remove undesired spatial and spectral components of light,

their reduced light transmission can affect the overall strength of the signal in optical systems, so their use should be carefully considered in applications where maximizing light throughput is essential for best results.

In summary, both slits and pinholes can serve as a spatial filter for a spectrometer. However, the slit as the first component of the spectrometer is more ideal for the RAID project. The spectrometer market also subtly supports this as all the other spectrometers reviewed earlier all use slits.

3.3.3 Lenses

The next component of the spectrometer that the light interacts with is a lens. Deciding on the lens is a lengthy process, given the plethora of types available in the market. It involves determining the best cost-effectiveness while also trying to keep the optical system as compact as possible. This lens's main job is to direct collimated light onto the grating surface. In this way, the lens contributes to ensuring that incident light strikes the grating at the proper angle of incidence - a critical component of effective diffraction.

This concentrated laser beam improves the grating's ability to disperse light at various wavelengths, which boosts the spectrometer's overall performance. Typically, coherent superposition of light waves or rays produces a wavefront. A wavefront is an imaginary surface that represents points in a wave that are in phase, or points that have the same phase angle/oscillation cycle. The application of the wavefront facilitates the visualization of the spatial distribution and how it changes as the light propagates through a medium and interacts with other optical components. Deviations from this flatness show aberrations or distortions in the wavefront, which can impair the performance quality of an optical system. A totally flat wavefront represents uniform and undistorted light propagation.

Furthermore, the lens is essential in regulating the form and size of the light beam that contacts the grating. To maximize the system's spectral resolution, this regulation is crucial. This makes it possible for us to accurately identify and analyze the spectral features like the Raman scattering peaks that are present in the light the enters the detector. The lens assists in reducing distortions and aberrations in the light beam prior to it reaching the grating. Aberrations can inject errors and artifacts into the spectrum that the spectrometer obtains, which could result in inaccurate results. The lens enhanced the spectroscopic measurements' overall accuracy and dependability by compensating for these aberrations.

The other lens in RAID’s optical system for the spectrometer goes after the light interacts with the grating. This is essential for ensuring effective light collection and detection as we must focus the diffracted light onto the photodiode. As we increase the signal intensity that is detected by the photodiode, we are also

improving the signal-to-noise ratio, Moreover, the spectrometer's sensitivity improves due to concentrating the scattered light onto a smaller region on the photodiode surface.

Moreover, the lens helps to reduce the problem of wavelengths diverging too far from the detector. Wavelengths diverge at different degrees when light disperses after going through the grating (chromatic dispersion). If remedial action is not taken, this divergence may cause wavelengths to miss the detector, resulting in distorted or incomplete spectral data to be analyzed. Strategically placing the lens to refocus the divergent wavelengths and send them towards the detector ensures that the detector receives the entire spectral range with the least amount of distortion or loss. Through the lens's correction of these spherical and chromatic aberrations, the detected spectrum is made to reflect the optical characteristics of the sample more accurately for analysis.

To start addressing these optical challenges, we began by looking at biconvex lenses. Sometimes referred to as a converging lens, the center of the convex lens is thicker than the edges. This results in the light rays that travel through it in parallel to converge at a focal point on the other side of the lens. Depending on the curvature, refractive index, and focal length of the lens we can determine the distance. Although this lens could be applied to our spectrometer when it comes to focusing the light onto the detector, having both edges of the lens the same creates more spherical aberrations. This is due to the paraxial and marginal rays are unable to focus on the same location. However, we can use a biconvex lens to create a wavefront. This is necessary for the lens in front of the grating. This can be seen below, and the cost of these are generally cheaper given their wide amount of applications:

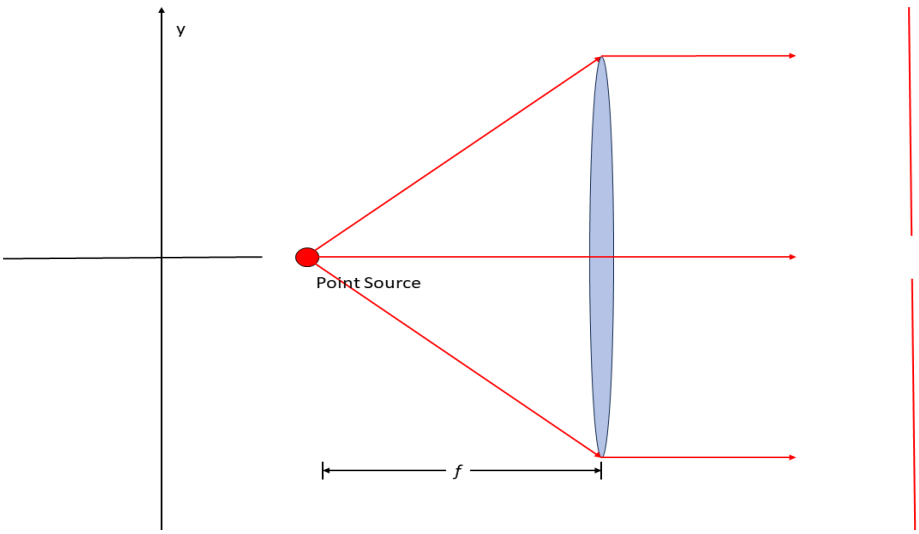


Figure 3.3.3 Biconvex Lens Creating Wavefront

Another lens to investigate is the plano-convex lens, which is characterized by one flat surface and one outwardly curved surface. Plano-convex lenses can converge incoming light rays into a focal point on the opposite side of the lens. Plano-convex lenses also have the benefit of being simple and straightforward to manufacture. Compared to more intricate lens designs, these lenses are comparatively simple to construct because they only have one curved surface. Because plano-convex lenses are simple to produce, they are an affordable option for us to take advantage of. By positioning the convex side towards the incoming beam of light, we can refract the rays with the curved side while limiting potential aberrations that may occur. In Figure (3.3. 3), we can see that the rays are not at the exact same location on the right image (due to the light exiting the curved side rather than the flat side, causing more erratic wavefronts to occur).

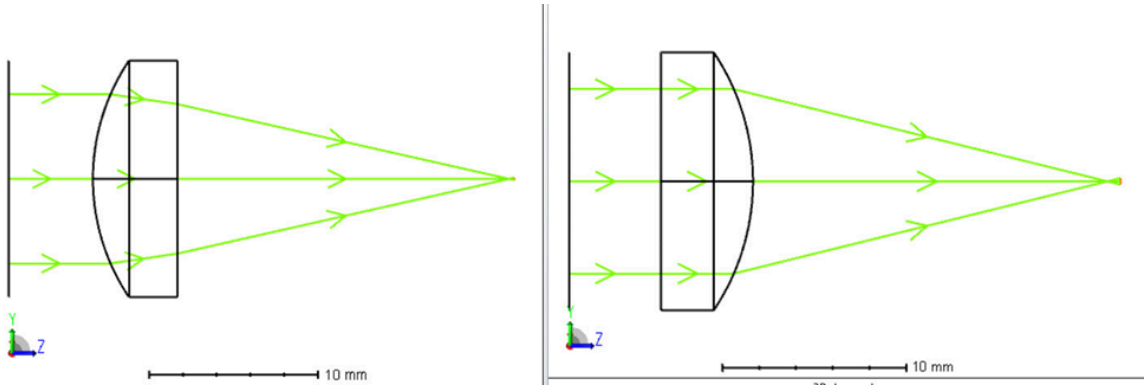


Figure 3.3.4 Propagation Effects Depending on Positioning of Lens (Found on Phystack Exchange)

A concave lens (known as diverging lens) has a thinner center than it does the edges. Being the opposite of a converging lens, the parallel light rays that travel through it become divergent as if they are emanating from a focal point behind the lens. This means we did not focus the light to a point but to a large surface area. This resulted in lowering the quality of the Raman spectra collected because we received less information (light). Moreover, the light rays do not collimate into a parallel beam as they keep diverging as it traveled to the grating.

A variation of this lens is known as a plano-concave lens, where one side is flat while the other is inwardly curved. Just like other concave lenses mentioned above, it diverges light rays away from a focal point. This could be useful since it does expand the beam onto a larger surface area. Although in the case of our set up, we decided to choose a photodiode as the detector which has a small area to detect with. This means that we could get away with a small beam being focused onto it.

Meniscus lenses with two types – positive and negative – have two spherical curved surfaces. One side of the lens is concave while the other side is convex.

From one perspective, a positive meniscus lens is concave, but when viewed from the other, it resembles a convex shape because it is thicker in the center than the corners. A negative meniscus lens, on the other hand, has a concave-convex profile and is thicker at the edges and thinner in the middle. These lenses can be used to collimate light, but due to their unique fabrication it comes at a higher cost ($500 or more) than other lenses. Before making a significant investment in collimating the light from the slit, we optimize other components first because there are more affordable solutions. Furthermore, it is often known that the plano-convex lens offers a better price-to-performance ratio.

3.3.4 Diffraction Grating

An optical element used to divide light into its component wavelengths is called a diffraction grating. It is made up of many parallel grooves or rulings that are closely spaced and usually etched or ruled onto a curved or flat surface. Light diffracts into different directions based on its wavelength when it comes into contact with a diffraction grating because of its interaction with the rulings or grooves. The concepts of wave interference and diffraction control this phenomenon.

Every single groove in the grating functions as a small slit, letting light flow through and diffract as it goes through. The angle at which light is diffracted into distinct wavelengths is determined by the distance between neighboring grooves. The diffraction equation states that the length of the grating and the wavelength of the light determine the angle of diffraction, with longer wavelengths diffracting at smaller angles and shorter wavelengths diffracting at larger angles.

The incident white light is divided into its constituent colors as a result of this diffraction process, creating a spectrum. Discrete spectral lines are produced when each wavelength of light is diffracted at an angle that is particular to the grating's characteristics. The grating surface's groove spacing determines the distance between these spectral lines; a broader color dispersion is produced by a closer distance, and vice versa. See the equation below:

$$d \cdot (sin\theta_m - sin\theta_i) = m \cdot \lambda$$

Equation 3.3.2 Grating Equation

This equation is the fundamental formula that controls how light is diffraction by a diffraction grating; this equation is sometimes referred to as the "grating equation." The grating surface's spacing between adjacent grooves is represented by d, the angle at which the m-th order spectral line is diffracted is indicated by θ_m, the angle at which incoming light is incident is indicated by θ_i, the order of diffraction (a positive or negative integer that indicates how many

times the light has been diffracted) is indicated by m, and the wavelength of light is indicated by λ. The path difference between consecutive grooves is represented by the left side of the equation, which multiplies the difference in the sine of the incidence and diffraction angles by the grating spacing. The path difference between consecutive grooves is represented by the left side of the equation, which multiplies the difference in the sine of the incidence and diffraction angles by the grating spacing.

In spectroscopy, diffraction gratings are frequently employed to examine the makeup of light sources. Scientists can identify the wavelengths present in the incoming light and the chemical components or molecules responsible for emitting or absorbing those wavelengths by measuring the angles and intensities of the spectral lines created by a diffraction grating. Diffraction gratings are also used in a variety of optical devices, including laser systems, monochromators, and spectrometers, where exact control over light dispersion is necessary to carry out tests or produce certain optical effects. All things considered, diffraction gratings are essential instruments in many fields of science and technology and are vital to our comprehension of how light behaves.

Due to these properties, the diffraction grating is one of the most essential optical components of the entire RAID system (specifically the spectrometer). This is because it serves as the fundamental element for dispersing light into its spectral components. The grating is designed with either rulings or grooves, which depends on whether the diffraction grating is holographic or ruled. The table below compares the two types of diffraction gratings that the RAID project team considered:

Table 3.3.2 Comparison of Holographic and Ruled Diffraction Gratings

Holographic Diffraction Gratings	Ruled Diffraction Gratings
Created by physically engraving (mechanically scribed) grooves onto the surface of the substrate material.	Created by using photoresist that is deposited onto a substrate. Light is exposed onto the optical interference pattern leaving a pattern.
Holographic gratings offer superior angular dispersion by virtue of their capability to inscribe extremely small period variations. They excel particularly in the ultraviolet range	Due to the inherent characteristics of the manufacturing process, ruled diffraction gratings invariably exhibit defects, such as periodic errors, spacing inconsistencies, and surface

and possess the added advantage of being inscribable onto curved surfaces, enabling not only angular dispersion but also focusing capabilities.	irregularities. These imperfections collectively result in heightened levels of stray light and ghosting, manifested as false spectral lines attributable to periodic errors.
Contain a sinusoidal cross-section, which poses challenges in achieving optimal blazing and often results in lower efficiency compared to ruled gratings of similar specifications. Exhibit reduced stray light compared to mechanically fabricated ruled gratings. This advantage stems from the absence of spacing errors inherent in ruled gratings, which tend to cause ghost reflections.	Ruled master gratings are specifically designed for applications in spectrometers and monochromators prioritizing cost-effectiveness and maximum efficiency. Ruled gratings surpass holographic ones in peak efficiency and offer a sharper spectral response centered around their blaze wavelength, attributed to their distinctive "sawtooth" groove profile.
Holographic diffraction gratings tend to be more expensive due to the intricate optical manufacturing processes involved, including precise control over interference patterns and specialized equipment requirements.	Ruled gratings are often more cost-effective compared to holographic gratings as they are typically mechanically ruled onto a substrate, requiring less complex manufacturing techniques and potentially lower material and equipment costs.

Ruled diffraction gratings stand out as an appealing option for a few reasons when compared using the table's comparison. First, they are economical without sacrificing effectiveness, which makes them perfect for uses where financial constraints are crucial. Ruled gratings' "sawtooth" groove profile allows for superior peak efficiency and spectrum responsiveness, especially at their maximum wavelength. Furthermore, although holographic gratings might provide better angular dispersion and less stray light, ruled gratings show less flaws and are more consistent and trustworthy in terms of performance. Their dependability and user-friendliness are enhanced by their simple manufacturing method, reduced vulnerability to recurring mistakes, and smoother surfaces. Overall, ruled diffraction gratings are a reasonable and practical option for a variety of spectroscopic and optical applications due to their affordability, efficiency, and dependability.

Higher line density diffraction gratings must be used to examine distinct spectrum segments, which increases light dispersion. As a result, less light overall enters the detector; yet this trade-off enables improved spectral resolution in the regions under analysis. The diffraction grating may also need to be adjusted when switching to a Raman experiment and changing the laser source. The Raman scattered light that reaches the detector varies depending on the wavelength of

the laser, even while Raman shifts for a sample are constant. In our case, we expect to see a Raman shift with a center wavelength at 580 nm. Therefore, we selected a laser at a nearby wavelength - 532 nm. On top of GABA's Raman shift, we chose this wavelength due to the 532 nm lasers being cheaper (high supply due to many applications).

Moreover, the Raman scattered light has closely spaced wavelengths due to the lower wavelength of the laser. For the light to be sufficiently dispersed across the detector, higher line density diffraction gratings are required. On the other hand, longer wavelength lasers scatter light more widely, necessitating the use of diffraction gratings with lower line densities for the best possible dispersion. It's important to recognize that gratings are fragile, especially given how frequently they may need to be replaced. Contact with solvents or even the oil from fingerprints can easily harm them. Therefore, to guarantee the durability and functionality of diffraction gratings in spectroscopic research, proper handling and maintenance procedures are essential.

Since it is one of the most expensive parts of our project, we must make sure it is accurate and appropriate right away. A mistake or oversight with the diffraction grating could cause serious problems for the experimentation process, thereby wasting data, resources, and time. Consequently, it is crucial to conduct in-depth study and give careful thought to elements like line density, dispersion characteristics, and laser source compatibility. Making the required time and effort up front to choose the right diffraction grating will reduce the possibility of expensive mistakes later and eventually increase the project's success and efficiency.

In addition to choosing between ruled and holographic gratings, we additionally must consider how to keep the Raman signal intact throughout the system. The RAID spectrometer must effectively catch and process the Raman signal once it interacts with the sample and disperses via the selected grating. This means choosing between a transmissive grating, which lets light pass through for additional analysis or collection, and a reflecting grating, which scatters incident light into its spectrum components and sends it towards a detector.

Table 3.3.3 Comparison of Transmissive and Reflective Diffraction Gratings

Transmissive Diffraction Gratings	Reflective Diffraction Gratings
Transmission gratings are generally less efficient when constructed with absorptive grooves, making them practical only up to approximately 1000 lines/mm. However, holographic transmission gratings offer an alternative approach, exhibiting spatial variation in phase	Reflective gratings, conversely, reflect all incident light while modulating only undesired light components. This characteristic contributes to their superior efficiency compared to transmission gratings. Reflective gratings excel in maintaining polarization, making them preferred for

rather than amplitude. Despite resulting in a different spectral behavior, these holographic gratings boast higher light throughput and efficiency.	applications where polarization preservation is crucial.
Spectral efficiency may be negatively impacted by some light loss via the grating, particularly in configurations where optimizing signal strength is crucial.	Effectively redirect incoming light in the direction of the detector to make the most of the available light and improve signal detection.
As the signal travels through the grating, it may attenuate or disperse slightly, which could affect the precision or strength of the signal that is detected.	Maintain the signal's integrity by guiding the scattered light toward the detector with the least amount of loss or distortion.
Usually have a "in-line" configuration, which leads to longer optical pathways. Because of this intrinsic design feature, transmission grating systems are less frequently used in configurations where optical compactness or space limits are important considerations. Instead, longer physical lengths are usually required.	Because they are common and flexible, reflection grating devices are often used in optical setups. Because they can diffuse and reflect light, they are preferred for their small and effective optical designs.
Since they let light through, they are perfect for systems that need to minimize optical distortion and maximize spectrum resolution, like imaging systems, fluorescence spectroscopy, and some forms of optical microscopy.	They are frequently used in configurations like Raman spectroscopy or some kinds of optical imaging systems, where the dispersion of light needs to be focused onto a detector or focal point for analysis.

Compactness is crucial for RAID's Raman spectrometer project, particularly for implementation in a bar environment. This criterion demands that every element—including the diffraction grating—be carefully considered. Reflective diffraction gratings are a desirable alternative because of the requirement for a small design. Their capacity to modulate undesirable components and reflect incident light efficiently guarantees maximum use of available space without sacrificing performance. Reflective gratings also preserve polarization, which is important for applications involving Raman spectroscopy. Their applicability is

further enhanced by their commonality and flexibility, which allows for the creation of small-sized but powerful optical equipment. Using reflecting diffraction gratings, RAID can create a Raman spectrometer that is portable, accurate, and efficient for on-site spectroscopic analysis—all necessary for meeting the needs of a bar environment.

In diffraction gratings, the phenomenon known as temporal dispersion is the variation in the delay time of optical pulses flowing through the grating according to the light's wavelength. various light wavelengths propagate through the grating at various rates, which causes this dispersion. The grating causes light of different wavelengths to diffraction, which causes the arrival times of the optical pulses to spread. The diffraction grating's design, the materials' optical characteristics, and the optical setup's geometry all affect how much temporal dispersion occurs. The formula for temporal dispersion with a diffraction grating is listed below:

$$\frac{1}{s} \cdot \frac{d\lambda}{d\tau}$$

Equation 3.3.3 Temporal Dispersion with a Diffraction Grating formula

This formula shows how the pulse delay time (τ) varies per meter of spacing between the gratings (s) with the wavelength of light (λ). In applications like the RAID project, where precise timing control of optical pulses is necessary for accurate spectroscopic measurements and data analysis, an understanding of and ability to manage temporal dispersion is critical.

The change in the angle of light diffraction as a function of wavelength is known as angular dispersion in diffraction gratings. Different light wavelengths are diffracted by varying amounts as they pass through the grating, which is caused by the dispersive nature of diffraction. The angle at which diffracted light is perceived varies in correlation with the wavelength of incident light. A diffraction grating's angular dispersion depends on several variables, including the order of diffraction, angle of incidence, and grating spacing. The formula for angular dispersion with a diffraction grating is listed below:

$$\frac{d\theta_m}{d\lambda} = \frac{m}{d^* cos\theta_m}$$

Equation 3.3.4 Angular Dispersion with a Diffraction Grating formula

This formula shows the relationship between the wavelength of light (λ) and the angle of diffraction (θ_m) for a particular diffraction order (m) and grating spacing (d). In spectroscopic applications, where exact understanding of how the diffracted light is spread across multiple wavelengths is necessary for correct measurement and analysis of spectral characteristics, it is imperative to comprehend and regulate angular dispersion.

In a diffraction grating configuration, the Littrow wavelength, sometimes called the Littrow condition, is a certain wavelength of light that meets a certain angle relationship. The diffraction angle of the same wavelength back into the same direction is equal to the incidence angle of light on the grating in the Littrow configuration, typically at 0th order (no diffraction). When the incident light, diffracted light, and the normal to the grating surface all lie in the same plane, this condition happens. The grating equation can be used to express the Littrow condition:

$$m * \lambda = 2 * d * sin(\theta)$$

Equation 3.3.5 Grating Equation for Littrow Condition

Since the angle of diffraction (θ) and the angle of incidence (θ) in the Littrow configuration are equal, the sine of the angle ($sin(\theta)$) equals 1. Consequently, the Littrow wavelength (λ_L) for a specific grating order (m) and grating spacing (d) can be computed as follows:

$$\lambda_L = \frac{2d}{m}$$

Equation 3.3.6 Littrow Wavelength equation

In the RAID project, the significance of the Littrow wavelength lies in its pivotal role within spectroscopy and optical design. This precise wavelength selection is critical in building the RAID spectrometer, guaranteeing that it can target and analyze certain spectrum properties important to our analytical goals. Furthermore, the Littrow wavelength is a key component in the construction of wavelength-selective optical systems adapted to our project's specific requirements, allowing for precise and dependable on-site Raman spectroscopy in a variety of environmental circumstances.

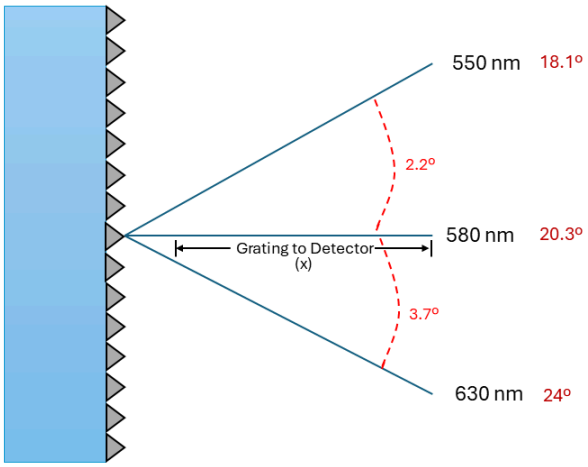


Figure 3.3.5 Range of Wavelengths and Angles Our Grating will Scan

Incorporating the Littrow formula, temporal dispersion formula, and the angular dispersion formula we determined a Littrow angle of about 20.365 degrees using a diffraction grating with 1200 lines per millimeter and a target center wavelength of 580 nm. We chose a diffraction grating with 1200 lines per millimeter since it is readily available and widely used in spectroscopic applications. The use of a regularly used grating specification provides various benefits, including ease of procurement, compatibility with conventional optical setups, and established performance characteristics. Moreover, it is a widely available grating to assure easy replacement and maintenance, as well as compatibility with other optical components.

The diffraction efficiency and dispersion properties are guaranteed to be optimum for the wavelengths of the laser excitation beam and the Raman spectral peak by using a grating with 1200 lines/mm. Within the spectroscopic setup, this line density allows for accurate wavelength selection and effective light collection by striking a compromise between spectral resolution and light throughput. We successfully obtained the Littrow wavelength of 580 nm, which is essential for our spectroscopic examination of the Raman shift peak of GABA. We were able to orient the diffraction grating in our spectroscopic setup perfectly thanks to this painstaking calculation, which guaranteed precision and peak performance while recording the relevant spectrum characteristics.

3.3.5 Detector Selection

When choosing a detector for a Czerny-Turner Raman spectrometer, several critical aspects must be examined to ensure optimal performance in detecting Raman scattered photons. The three most important characteristics in this selection procedure are Noise Equivalent Power (NEP), active area, and sensitivity. NEP (watts per square root of hertz) measures the detector's minimal detectable power level. It represents the detector's signal-to-noise ratio and its capacity to separate weak signals from background noise. A lower NEP value gives us greater sensitivity and efficacy in detecting feeble Raman signals among noise.

The active area is the physical area of the detector that is responsive to incident light. In Raman spectroscopy, a larger active area is preferable because it allows for the capture of more photons scattered by the sample, resulting in a stronger signal. However, it is critical to achieve a balance between active area size and detector size, as larger detectors may inject additional noise or complexity into the optical system. As a result, choosing a detector with a suitably sized active area customized to the individual experimental requirements is critical for maximizing signal collection efficiency while maintaining system performance.

In Raman spectroscopy, achieving the maximum possible sensitivity while minimizing noise is critical, as identifying weak Raman signals against a background of noise can be difficult. Sensitivity relates to the detector's ability to detect minor changes in light intensity, which is commonly measured in terms of electrical output per unit of incident light power. In the RAID project, sensitivity is crucial for improving the signal-to-noise ratio and the spectrometer's detection limit given how small our GABA signals are. However, it is important to establish a balance between sensitivity and noise levels, as detectors that are too sensitive can magnify the noise alongside the signal, reducing the quality of the spectrum data (signal and noise become indistinguishable).

In conclusion, when choosing a detector for a Czerny-Turner Raman spectrometer system, it is critical to consider metrics such as NEP, active area, and sensitivity. By selecting a detector with a low NEP, a suitable active area, and balanced sensitivity, we ensured efficient detection of Raman signals with a high signal-to-noise ratio, allowing for accurate and consistent measurements of GABA Raman signals being detected.

A photodiode is a semiconductor device that converts light into electricity via the photovoltaic effect or photoconductivity. It consists of a p-n junction, where photon absorption forms electron-hole pairs, causing current to flow. Photodiodes are widely utilized for a variety of applications, including optical communication, light detection, and spectroscopy. In the RAID project, a photodiode can be used for detecting Raman scattered light from the sample being analyzed. When a laser beam illuminates a sample (GABA in liquid), it produces Raman scattered photons with wavelengths that match to the molecules' vibrational modes. These

photons are gathered and focused on the photodiode, producing electrical impulses proportional to the intensity of the dispersed light. The photodiode detects and measures these signals, allowing the RAID spectrometer to capture the sample's Raman spectra, which provide significant insights into its molecular composition and structure.

An avalanche photodiode (APD) is a type of photodiode that operates with a high reverse bias voltage. Unlike typical photodiodes, APDs use an internal avalanche multiplication process in which a single electron-hole pair produced by input photons initiates a cascade of secondary electron-hole pairs by impact ionization. This multiplication process increases the initial photocurrent, resulting in greater sensitivity and lower noise levels than ordinary photodiodes. In the RAID project, an avalanche photodiode was used to improve sensitivity and detection efficiency, for as when examining samples with weak Raman signals or in low-light settings.

A CCD (Charge-Coupled Device) is a specialized image sensor that is widely used in digital cameras and imaging systems. It is made up of an array of small capacitors, each of which may store the electrical charge generated by incident photons. When light strikes the CCD array, it produces a charge proportionate to the intensity of the incident light at each pixel. The accumulated charge is then progressively read and translated into digital signals, resulting in an image representation of the scene. In spectroscopy, CCDs are frequently used as detectors to capture spectral data. In the RAID project, a CCD may be utilized instead of a photodiode or avalanche photodiode to detect Raman scattered light.

Finally, a linear array detector is a form of sensor made up of several photodetectors organized in a linear array pattern. Each photodetector element in the array represents a specific wavelength range or spectral band. Linear array detectors are widely employed in spectroscopic devices to collect one-dimensional spectrum data. In the RAID project, a linear array detector can be used to capture Raman spectra in a more compact and cost-effective manner than CCDs. By organizing numerous photodetectors in a linear array, the detector may capture spectral data across a wide range of wavelengths at the same time, allowing for the quick acquisition of Raman spectra with high resolution. Furthermore, linear array detectors provide benefits such as simplicity, dependability, and interoperability with tiny spectroscopic systems, making them ideal for on-site Raman spectroscopy applications in situations such as bars.

The table below compares the four detectors we considered using for the RAID spectrometer:

Table 3.3.4 Comparison of Detection Components

Parameters	Photodiode	Avalanche Photodiode	CCD	Linear Array
Price	Relatively Inexpensive (~$20)	Moderate to Expensive (~$50 - $200)	Expensive (~$200 - $600)	Expensive (~$200 - $600)
Performance	Good Sensitivity (400 – 1000nm), fast response time	Good Sensitivity (450 – 1000 nm), fast response time	Good Sensitivity (400 – 1000 nm), fast response time	Good Sensitivity (400 – 1000nm), fast response time
Flexibility	Compact and versatile, can be easily integrated into various optical setups	Compact and versatile, can be easily integrated into various optical setups	May constrain system design due to size and integration requirements	May require a stationary configuration, but compatible with moving diffraction grating if integrated properly
System Constraints	Minimal constraints, compatible with moving components such as a moving diffraction grating	Minimal constraints, compatible with moving components	May constrain system design due to size and integration requirements	May require a stationary configuration, but compatible with moving diffraction grating if integrated properly
Spectral Range	190 to 1000 nm	200 to 1150 nm	200 to 1100 nm	350 to 1000 nm
Pixel Size	N/A	N/A	6 – 25μm	N/A
Quantum Efficiency	40 – 90%	75%	80 – 90%	70 – 90%
Start Time	Short	Short	Slightly Longer	Short

Low Dark Current?	✔	✔	✔	✔
Linearity?	✔	✔	✔	✔
Cooling Requirements	N/A	N/A	Typically needed for optimal performance	Not necessary, but could benefit from cooling depending on application
NEP ( ) For when ( )				
Sensitivity (A/W)	0.35 – 0.50	0.40 – 0.50	0.3 – 0.7	0.50 – 0.72 (larger area)
Active Area	Small	Small	Medium to Large	Medium to Large

After carefully assessing the parameters given in the comparison table, various reasons contribute to the strategic advantage of including an avalanche photodiode (APD) into the RAID project's Czerny-Turner Raman spectrometer system, in addition to its technical qualities. By using an APD, the project benefits from its high sensitivity and quick response time, which are critical for detecting weak Raman signals with precision and efficiency. Moreover, the introduction of an APD fits neatly into the spectrometer's design, allowing for the integration of a stepper motor to regulate the movement of the diffraction grating. This integration improves the operational workflow by efficiently spreading task demands among project teams. By choosing an APD, the RAID project may effectively balance performance, resource utilization, and cost efficiency, assuring the best solution for its spectroscopic needs while maximizing project resources.

Furthermore, the decision to use an APD is influenced by practical and budgetary issues in addition to technical ones. While linear arrays and CCDs improve measuring performance, their use adds complexity and cost to the project. APDs, on the other hand, offer a low-cost option while maintaining measuring accuracy and sensitivity. This strategic decision allows the project to spend resources more efficiently, increasing value while keeping a strong spectroscopic capacity. In essence, by exploiting the benefits of an APD, the RAID project achieves a balance between technical excellence, operational efficiency, and budgetary prudence, ensuring the effective realization of its spectroscopic objectives within the restrictions of its resources and timeframe.

3.4 Rotating Stage

Grating rotation plays a crucial role in the operation of Raman spectrometers, particularly those utilizing dispersive spectrometry. It is a fundamental mechanism that enables the analysis of Raman scattered light across a range of wavelengths, providing valuable insights into the molecular composition and structure of a sample.

In a Raman spectrometer, the grating serves as a crucial component for dispersing the Raman scattered light according to its wavelength. The grating should be positioned in the path of the scattered light, and as the light passes through the grating, it is diffracted at different angles depending on its wavelength. By rotating the grating, the spectrometer we scan through different wavelengths of the Raman scattered light, allowing for the measurement of the complete Raman spectrum.

The grating rotation mechanism is typically motorized and controlled by the spectrometer's software. The software specifies the angle and speed of rotation, ensuring precise control over the scanning process. This precise control is essential for obtaining accurate and reproducible Raman spectra.

Grating rotation offers several advantages in Raman spectrometry. By scanning through different wavelengths, it allows for the identification of specific molecular bonds and functional groups in a sample. This information is crucial for various applications, including material characterization, pharmaceutical analysis, and environmental monitoring.

It is important to note that while grating rotation is a powerful technique, it is not without its challenges. One of the main challenges is maintaining the alignment and stability of the grating during rotation. Any misalignment or instability lead to errors in the spectral data. Additionally, the speed of rotation must be carefully controlled to ensure that the spectral data is collected at a consistent rate.

Grating rotation is used in a wide range of spectroscopic applications, including Raman spectroscopy, fluorescence spectroscopy, and atomic absorption spectroscopy. In Raman spectroscopy, it is particularly valuable for studying complex samples with multiple molecular components, where the ability to scan through different wavelengths provides detailed information about the sample's composition and structure.

In conclusion, grating rotation is a fundamental technique in Raman spectrometry, enabling the measurement of the complete Raman spectrum and providing valuable insights into the molecular composition and structure of a sample. Its precise control and versatility make it a valuable tool for researchers

and spectroscopy enthusiasts seeking to explore the intricacies of molecular interactions.

3.4.1 Rotating Stage Selection

After identifying our criteria, we focused our search on three rotating stages available in the market: Thorlabs RSP1, Thorlabs XRR1, Newport URS50B. We will now explore the key advantages and challenges of each stage and present a table to visually compare their features.

3.4.1.1 Thorlabs RSP1

The Thorlabs RSP1 is a compact and affordable manual rotating stage commonly used in optical setups for precision angular positioning. With a diameter of 1", this stage provides smooth rotation with a resolution of 1°, making it suitable for various applications requiring precise angular adjustment, such as aligning optical components like mirrors, filters, and lenses. The RSP1 features a removable knob for convenient adjustment and a locking screw to secure the stage in place once the desired position is achieved. Its compact design and compatibility with standard optomechanical components make it an ideal candidate for compact setup such as a Raman spectrometer. However, one limitation of the Thorlabs RSP1 is its manual operation, which may require more effort and time compared to motorized stages, especially for applications requiring frequent and precise adjustments. Additionally, the resolution of 1° may not be sufficient for applications requiring very fine angular positioning. Despite these limitations, the Thorlabs RSP1 remains a popular choice among researchers and engineers for its affordability, reliability, and compatibility with a wide range of optical components.

3.4.1.2 Thorlabs XRR1

The Thorlabs XRR1 is a high-precision rotation stage designed for demanding optical and mechanical applications. It features a large 1.5" (38.1 mm) clear aperture, allowing for the passage of light or other elements through the stage. The XRR1 offers a 360° continuous rotation with a resolution of 0.005°, providing precise angular positioning for alignment and measurement tasks. One of the key advantages of the XRR1 is its high precision and repeatability, making it suitable for applications requiring accurate angular positioning, such as in optical interferometry, microscopy, and laser processing. The stage is also equipped with a locking mechanism to secure the stage in place once the desired position is achieved, ensuring stability during measurements or alignments.
The XRR1 also features a compact and modular design, allowing it to be easily integrated into existing setups or customized for specific applications. The stage is compatible with a range of accessories, such as optical mounts and actuators, further enhancing its versatility.

3.4.2 HT03RA100

The HT03RA100 is a high-precision rotary stage manufactured by Hiwin Corporation, designed for precise angular positioning in various applications, including optical setups and industrial automation. With a diameter of 100 mm, this stage offers a high load capacity and smooth rotation, making it suitable for applications requiring the positioning of heavy or delicate components with high precision. The HT03RA100 features a precision ground worm gear mechanism, providing high accuracy and repeatability in angular positioning. It also includes a locking mechanism to secure the stage in place once the desired position is achieved. One advantage of the HT03RA100 is its high load capacity, which allows it to handle heavier loads compared to smaller stages. Additionally, the precision ground worm gear mechanism ensures smooth and precise rotation, making it suitable for applications requiring high precision and repeatability. However, one limitation of the HT03RA100 is its relatively larger size, which may require more space in the setup compared to smaller stages. Despite this, the HT03RA100 is a popular choice among researchers, engineers, and manufacturers who require a high-precision rotary stage for demanding applications.

Table 3.4.1 Rotation Stage Comparison

Feature	**Thorlabs RSP1**	**Thorlabs XRR1**	**Hiwin HT03RA100**
Clear Aperture	1" (25.4 mm)	1.5" (38.1 mm)	-
Angular Resolution	1°	0.005°	-
Motor Type	Manual	Manual	Precision Ground Worm Gear
Motorized	No	No	No
Load Capacity	-	-	High
Locking Mechanism	Yes	Yes	Yes
Compatible with Arduino	No	No	No
Application Suitability	Basic angular positioning	High precision applications	Heavy-duty applications

Price Range	98.42	480.54	349.99

3.4.2.1 Custom Rotating Stage

Between affordability and limited options for motorized stages, we decided to design and assemble a motorized stage for our project. We will now explore the components needed to build a custom motorized stage. Designing our motorized stage will allow us to customize the stage to fit the specific grating lens, load capacity, and speed of rotation. This level of customization can be hard to find in off-the-shelf products.

To design said motorized stage we will need a stepper motor, which provides precise rotational control, NEMA 17, NEMA 14. The selected motor will need to be paired with a stepper motor driver to control its movement. We will explore between the A4988 and the DRV8825. Additionally, we will need a platform for the diffraction grating, which can be 3D printed or made from acrylic or wood. The platform should be mounted on bearings to reduce friction and ensure smooth rotation. The stepper motor and driver can be controlled by a microcontroller such as an Arduino or MSP430fr6989, which can be programmed to send the necessary commands for rotation.

3.4.3 Stepper Motor Driver

3.4.3.1 A4988

The A4988 is a popular stepper motor driver used in various DIY and industrial projects. It is manufactured by Allegro Microsystems and is widely used due to its simplicity and reliability. The A4988 can drive bipolar stepper motors with up to 2A per phase and operating voltages between 8V and 35V. It features adjustable current limiting, overcurrent and overtemperature protection, and five different step resolutions (full, half, quarter, eighth, and sixteenth steps). These features make the A4988 suitable for applications requiring precise control over stepper motors, such as 3D printers, CNC machines, and motorized stages for scientific instruments like Raman spectrometers.

3.4.3.2 DRV8825

The DRV8825 is another popular stepper motor driver, manufactured by Texas Instruments. Like the A4988, it is widely used in DIY and industrial projects for its performance and reliability. The DRV8825 can drive bipolar stepper motors with up to 2.5A per phase and operating voltages between 8.2V and 45V. It offers adjustable current limiting, overcurrent and overtemperature protection, and up to 32 micro-step resolutions (full, half, 1/4, 1/8, 1/16, 1/32 steps). The DRV8825's

higher micro-stepping capability compared to the A4988 makes it suitable for applications requiring smoother motion and higher resolution, such as precision instruments and robotic systems.

Originally the DVR8825 was chosen for this project but halfway through the project we quickly realized that the DVR8825 did not our demand. We needed the rotating stage to micro-step 0.005 (+/- 0.001) degrees and between the chosen gears' ratio and the up-to-1/32 micro-step of the stepper driver, we were only able to achieve 0.0085 degrees. The original gears chosen were a 13T 32P pinion gear driving a 86T 32P gear which provided an 86/13 = 6.615 gear ratio. By default, the NEMA 14 takes 1.8 degrees steps. The DVR8825 allows up to 32 micro-steps which makes the effective micro-step 1.8/32 = 0.056, leaving the final step to be 0.056/6.6.615 = 0.0085 which did not meet our requirement. After further research, we chose the TCM2209 which allowed 1/256 micro step through UART.

Table 3.4. 2 Stepper Motor Driver Comparison

Feature	A4988	DRV8825	TMC2209
Manufacturer	Allegro MicroSystems	Texas Instruments	Trinamic
Max Current per Phase	2A	2.5A	2A (peak current up to 2.8A)
Operating Voltage	8V - 35V	8.2V - 45V	4.75V - 29V
Micro-stepping	Full, Half, 1/4, 1/8, 1/16	Full, Half, 1/4, 1/8, 1/16, 1/32	Full, Half, 1/4, 1/8, 1/16, 1/32, 1/256
Overcurrent Protection	Yes	Yes	Yes
Overtemperature Protection	Yes	Yes	Yes
Step Resolutions	Full, Half, 1/4, 1/8, 1/16	Full, Half, 1/4, 1/8, 1/16, 1/32	Full, Half, 1/4, 1/8, 1/16, 1/32, 1/256
Suitable Applications	General purpose projects	Projects requiring higher resolution	Projects requiring ultra-silent operation
Compatible with Arduino	Yes	Yes	Yes
Compatible with MSP430FR6989	Yes	Yes	Yes
Price	12.99	13.49	~15.00

3.4.4 Stepper Motor

3.4.4.1 NEMA 17

The NEMA 17 stepper motor is popular in DIY and industrial applications. It provides a small footprint mounting flange size of 1.7 x 1.7 inches. The NEMA 17 is known for its compact size and high torque output, making it suitable for a wide range of applications. One of the key features of the NEMA 17 stepper motor is its high step resolution, which allows for precise control over its rotation. This makes it ideal for applications such as 3D printers, CNC machines, camera sliders, and robotics, where precise positioning is crucial. The NEMA 17 stepper motor typically has a step angle of 1.8 degrees, meaning it takes 200 steps to complete a full revolution. However, micro-stepping can be used to achieve even finer resolutions.

3.4.4.2 NEMA 14

The NEMA 14 stepper motor is a compact stepper motor known for its small size and moderate torque output. The NEMA 14 stepper motor is used in applications where space is limited and precise control over movement is required, it offers a footprint of 1.4 x 1.4 inches. This makes it suitable for applications such as small robots, cameras, and medical devices where space is a constraint. The NEMA 14 stepper motor typically has a step angle of 1.8 degrees, meaning it takes 200 steps to complete a full revolution. In terms of specifications, the NEMA 14 stepper motor is available in various lengths and holding torques, ranging from around 0.15 Nm to 0.35 Nm. It operates at voltages typically ranging from 3V to 12V, although this can vary depending on the specific model. The smaller footprint of the NEMA 14 makes it ideal for our projects.

Table 3.4.2 Stepper Motor Comparison

Feature	**NEMA 17**	**NEMA 14**
Mounting Size	1.7 x 1.7 inches (NEMA 17)	1.4 x 1.4 inches (NEMA 14)
Torque Output	Higher	Lower
Step Angle	1.8 degrees	1.8 degrees

Voltage Range	3V - 12V	3V - 12V
Price Range	$10 - $30 (approx.)	$5 - $20 (approx.)
Arduino Compatibility	Yes	Yes
MSP430FR6989 Compatibility	Yes	Yes

Our final configuration for our motorized rotating stage is a TCM2209 stepper driver paired with a NEMA14. The TCM2209 is set to 1/64 micro-step leaving the effective step to be 1.8/64 = 0.0281 degrees. With this motor setup up the previously chosen gears/gear ratio would have met our requirement however the 32P gears allowed some backlash that made the rotating stage micro-steps unreliable. To compensate for this error, we chose a 48P gear set/ with more teeth per inch the backlash was eliminated. Our final configuration is a 20T 48P gear pinion driving a 90T 48P gear, giving us a 4.5 gear ratio. Leaving our final effective step to be 0.0281/4.5 = 0.00625.

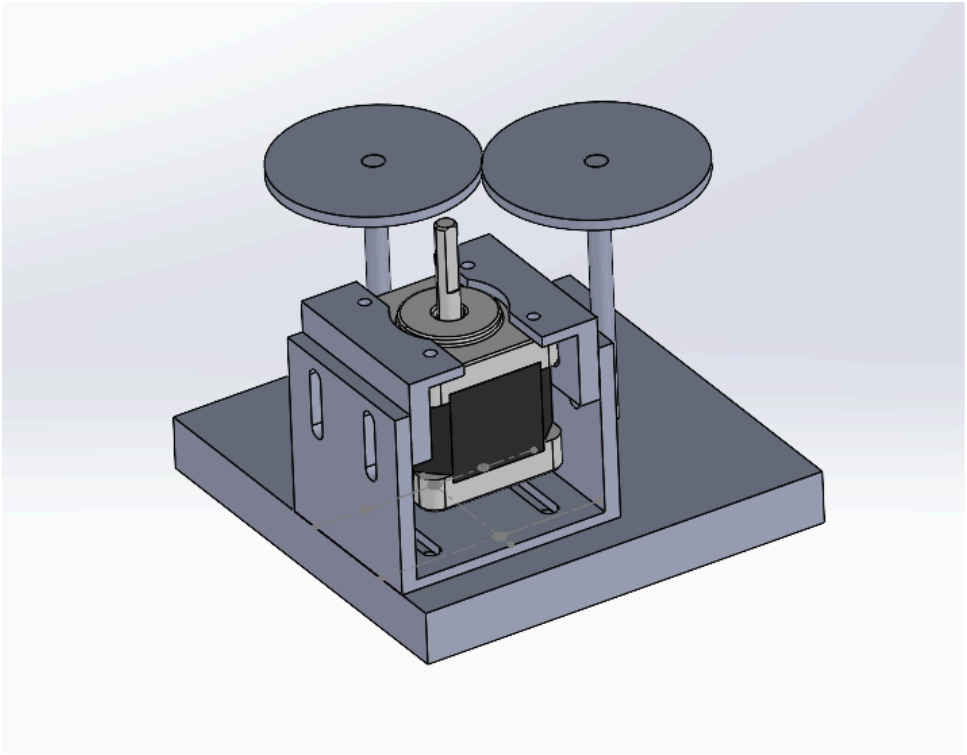


Figure 3.4.2.1 Motorized Stage

3.5 Microcontroller

A microcontroller is a compact, single integrated circuit designed or optimized for a specific application or operation within an embedded system. Single integrated systems such as these are usually comprised of programmable input/output peripherals, a processor core, and memory (The Mechatronics Blog, 2024).

Microcontrollers are highly useful devices due to their unique capabilities and features tailored for embedded systems and applications. According to ChatGPT's OpenAI platform there are a multitude of reasons as to why microcontrollers are so valuable:

1. Integration of Components: Microcontrollers are compact integrated circuits that combine a processor (CPU), memory (RAM and ROM), input/output peripherals (GPIO - General Purpose Input/Output), timers, and communication interfaces (such as UART, SPI, I2C) into a single chip. This integration makes them ideal for applications where space, power consumption, and cost are critical factors.

2. Efficiency and Cost-Effectiveness: Compared to using separate components (like discrete processors, memory, and peripherals), microcontrollers are more efficient and cost-effective. They reduce the PCB (Printed Circuit Board) size, simplify the design, and decrease the overall system cost.

3. Low Power Consumption: Microcontrollers are designed to operate efficiently within limited power budgets, making them suitable for battery-powered and energy-conscious applications. They can be put into low-power sleep modes and wake up in response to external events, extending battery life.

4. Real-time Processing: Many microcontrollers are equipped with built-in peripherals like timers, PWM (Pulse Width Modulation) controllers, and ADCs (Analog-to-Digital Converters) that enable them to handle real-time tasks and interact with the physical world in ways that traditional computers cannot.

5. Customizability and Flexibility: Microcontrollers can be programmed to perform specific tasks tailored to the requirements of the application. This flexibility allows developers to optimize performance, reduce unnecessary overhead, and implement custom functionalities.

6. Wide Range of Applications: Microcontrollers are used in various industries and applications, including consumer electronics (like smart home devices, wearable technology), industrial automation (such as robotics and process control systems), automotive electronics (like engine control units and dashboard

displays), medical devices (like implantable devices and diagnostic tools), and more.

7. Ease of Prototyping and Development: Microcontrollers are often supported by a wealth of development tools, including integrated development environments (IDEs), compilers, debuggers, and simulation software. This ecosystem facilitates rapid prototyping and iterative development cycles.

8. Availability of Libraries and Resources: Microcontroller manufacturers and the open-source community provide extensive libraries and resources that simplify complex tasks such as interfacing with sensors, handling communication protocols, and implementing advanced algorithms.

9. Reliability and Durability: Microcontrollers are designed to operate reliably in harsh environments (e.g., extreme temperatures, vibration, and humidity), making them suitable for use in rugged applications.

10. Scalability: Microcontrollers come in a range of specifications and capabilities, from simple 8-bit controllers to advanced 32-bit processors with extensive memory and peripheral options. This scalability allows developers to choose the right microcontroller for their specific needs without overdesigning or underperforming (OpenAI, 2024).

In Raman spectrometry, microcontrollers play a vital part in the operation of the spectrometer as they serve as the central processing unit or command center of embedded system controlling functions of a spectrometer's operation including but not limited to laser control, optical system control, data acquisition, signal processing, spectrum analysis, user interface, system monitoring and diagnostics, as well as data logging and communication and are typically controlled by the laser system's driver circuit.

Regarding data acquisition and processing, scattered light from a sample is analyzed by the spectrometer to identify the molecular composition. This process is managed by triggering and controlling the lasers, overseeing the spectrometer's optical components, compiling spectral data, and capturing the resulting spectra.

To guarantee optimal system performance and accurate results in Raman spectroscopy, real time control is another element that must be taken into consideration. The microcontroller allows for data processing in real-time with the ability to adjust aspects like laser power, integration time, and spectral range based on feedback from the spectrometer's detectors.

Microcontrollers are also in charge of communication and coordination between peripheral devices such as motors, light sources, detectors, and user interfaces to establish successful operation of the Raman spectroscopy system. In Raman spectroscopy, a microcontroller can serve as the central processing unit that controls various aspects of the system, from data acquisition to signal processing and interpretation.

One key application of microcontrollers in Raman spectroscopy is managing the interface with the spectrometer components, including lasers, detectors, and optical filters. The microcontroller can coordinate the timing and synchronization of these components, ensuring precise control over the excitation and detection processes critical for Raman measurements. Using microcontrollers allows for real-time data retrieval and processing in order to analyze spectral data directly on the device. This capability is particularly valuable for portable or field-deployable Raman systems where computational resources are limited. Microcontrollers are also beneficial for implementing algorithms for background subtraction, spectral calibration, and pattern recognition, enhancing the accuracy and reliability of Raman spectroscopy measurements.

Many Raman spectrometers are often used in portable devices or field applications making power efficiency and compact design important features to consider. They are designed for their minimal power consumption and compact capabilities, serving as a great component for applications that have a heavy focus on space and energy efficiency. Overall, integrating microcontrollers into Raman spectroscopy systems not only streamlines operation and improves performance but also enables the development of compact, cost-effective, and user-friendly instruments for various scientific, industrial, and biomedical applications.

In conclusion, the microcontroller is a key piece in Raman spectroscopy as it controls the data acquisition process, facilitates user interaction, processes spectral data, and monitors the reliability and accuracy of the results. Its integration enables the automation, precision, and versatility required for advanced Raman spectroscopy applications.

3.5.1 Microcontroller Market Comparison

The microcontroller market is vast and continuously expanding, driven by increasing demand for smart and connected devices across multiple industries. Microcontrollers are widely used in consumer electronics, automotive systems, industrial automation, healthcare devices, and IoT (Internet of Things) applications. Major players fueling the growth of this market include advancements in semiconductor technology leading to more powerful and

energy-efficient microcontrollers, rising adoption of automation and digitalization, and the proliferation of IoT devices requiring embedded processing capabilities. The market is characterized by a diverse range of options for microcontrollers, from low-cost, low-power 8-bit controllers suitable for simple applications to high-performance 32-bit microcontrollers with advanced features for complex tasks. As emerging technologies such as AI (Artificial Intelligence) and edge computing become even more popular, microcontrollers are expected to play an even larger role in shaping the future of connected devices and smart systems.

Based on the criteria discussed above, we narrowed down our search to three microcontrollers available on the market: ST Microelectronics 32 Nucleo-F401RET6 Microcontroller, Raspberry Pi 3 Model B+, and Arduino Uno. The features, advantages, and disadvantages of each will be disclosed and present via a table for display.

3.5.1.1 ST Microelectronics 32 Nucleo-F401RET6 Microcontroller

The ST Microelectronics 32 Nucleo-F401RET6 is a development board based on the STM32F401RET6 microcontroller which is built around ARM Cortex-M4 core for low power applications. With GPIO pins, USB Arduino Rev 3 connectivity, 512 KB of RAM, SPI, I2C, and many other peripheral interfaces, there are many features on this board (The Mechatronics Blog, 2024). Like the Arduino board the STM 32 Nucleo boards provide flexibility and customization to achieve specific requirements of the Raman spectrometer. However, there are potential drawbacks to this board including limited processing power and memory, development complexity, and compatibility with the peripheral. All in all, though at the price of $13.83 this board seems as if it will be able to perform the necessary tasks needed to complete the Raman spectroscopy experiments including basic analysis, data acquisition, high performance, flexibility, and real time control.

3.5.1.2 Raspberry Pi 3 Model B+

The Raspberry Pi 3 Model B+ is a single board computer developed by Raspberry Pi Foundation used for a variety of applications from automation and robotics to educational experiments. It features 1.4 GHz with 64-bit quad core ARM Cortex-A53 processor, 1 GB of RAM, numerous I/O ports, GPIO pins, and built-in wireless connectivity options (Pololu, 2024). This Raspberry Pi model offers more computing power compared to the Arduino or STM32 models thanks to its quad-core ARM processor and 1 gigabyte of RAM allowing for it process and handle more data processing tasks contributing to real time analysis of Raman spectroscopy experiments. Raspberry Pi 3 Model B+ presents itself as both a powerful and versatile option for microcontrollers as it relates to Raman spectroscopy as its features balance the key aspects needed including data

acquisition, real time analysis, flexibility, and affordability making it a solid choice for building a Raman spectrometer.

3.5.1.3 Arduino Uno

The Arduino Uno is a popular microcontroller board primarily for beginners, based on the Atmega328 microcontroller acting as the base of operations for the board. Features of the board include a USB connection, 16 MHz quartz crystal, 14 digital I/O pins – 6 of which can be used as Pulse Width Modulation outputs, and 6 analog input pins. A USB interface allowing communication between the microcontroller and computer is included to upload code and transmit data to and from other devices. The USB also can be used as a power supply in addition to the external power supply connected via DC power jack which is ideal for portable projects. A board like this is primarily used for educational purposes such as at home projects or workshops for beginners. A microcontroller such as this would only be able to handle minimal data transmission like relaying sensor information not complex data analysis or acquisitions. Although this microcontroller has a decent price of $24.99, the drawback of having potentially delayed real time results is not a worthy or fair tradeoff.

Table 3.6.1 Microcontroller Comparisons

Features	STM32 Nucleo-F401Rpy ET6	Raspberry Pi 3 Model B+	Arduino Uno
Processor	Cortex-M4 core, up to 84 MHz	1.4 GHz 64-bit quad core	16 MHz
RAM	512 KB	1 GB	8 KB SRAM
Drive Space	512 KB Flash	32 GB Flash	32 KB Flash
Input Voltage	3.3 - 12 V	5.1 V	12 V
Dimensions	4” x 3” x 1”	3.7” x 2.8” x 1.14”	3.15” x 2.17” x 0.98”
Weight	3.2 oz	7.1 oz	1.6 oz
Other features	GPIO pins, USB, Arduino Uno Rev 3 connectivity	Extended 40-pin GPIO header, USB	14 DIO Pins, USB

Pricing	$13.83	$46	$24.99

Microcontroller Final Selection

Based on the research conducted as shown in the table above the microcontroller chosen for this project was the Raspberry Pi 3 Model B+. In comparison to the other microcontroller options the Raspberry Pi 3 Model B+ is the most cost-effective while balancing the factors of connectivity, processing power, operating system support, memory and storage, as well as providing community support for users with tutorials and documentation provided for any troubleshooting that may be necessary when building the Raman spectrometer.

3.6 Screen Display

In a Raman spectrometer, a screen display plays more of an optional role in comparison to other instruments involved as it is not directly related to data analysis techniques but more so helpful for data visualization or the user interface. In RAID's case, the screen display would display the results of illicit drug detection using a color system: red, yellow, or green and would be controlled by the microcontroller. Red meaning negative, yellow meaning undetermined, and green representing positive. Many modern Raman spectrometers today have a screen display to show important information such as instrument settings, spectral data, real-time monitoring, and calibration information.

With a screen display, users have the advantage of being able to view and adjust instrument settings like spectral resolution, integration time, laser wavelength, and/or other parameters.

Spectral data from the Raman spectrum scan may be shown via the display of a graph showing a Raman shift on the y-axis for intensity or x-axis for wavelength. Molecular vibrations and characterizations can be made and identified by this data analysis.

The screen display can also provide real-time monitoring by granting users the ability to review signal quality and make modifications as needed based on the feedback of the progress of the measurement during a scan.

Important calibration information regarding status and curves from the Raman spectroscopy analysis may be shown on the screen to certify that there are accurate measurements.

Many Raman spectroscopy display screens have advanced features specifically designed for precise analysis and visualization of data providing both chemical and structural data to the user. These screens are typically comprised of multi-mode display options such as 2D and 3D representations with the inclusion of user-friendly interfaces powered by advanced software to generate and facilitate real-time spectral acquisition and processing. Key aspects like high-resolution screens and fast response times are to be expected from these machines. Other features may include interactive tools for spectral data comparison and peak identification which allows for efficiency regarding research and analysis as well as real time feedback on sample results and characteristics.

The use of these customizable display screens is meant to serve the purpose of successfully optimizing the visualization and interpretation of spectral data in order to create a tool for powerful analysis.

Raman spectrometers involving displays can pose their challenges because of the fluorescence emitted when they are powered on. Spectral artifacts and reduced sensitivity when attempting to detect Raman signals from the sample are possible based on this fluorescence as this interferes with Raman signals. To minimize these effects, spectral subtraction techniques and instruments to compensate for any fluorescence present must be used. There are several types of screens displays we can consider when choosing one for our Raman spectrometer with the most popular being discussed below.

The most popular screen display types:

- LCD
- LED
- OLED
- Mini-LED

A liquid crystal display (LCD) is a flat panel display that uses modulated light through liquid crystals to produce text or images on a screen in modern electronics. LCD display screens are composed of several components to generate text and/or images including backlight, polarizing filters, liquid crystal layer, thin-film transistors, color filters, glass or plastic substrates, and driver electronics (TechTarget, 2024). Two layers of polarized glass hold liquid crystals that control light that passes through to generate text, images, or videos using vivid color and detail. Pros for this display technology include its sharp image quality, range of brightness levels, and high resolution resulting in pristine visibility even in the brightest places. Recent advancements even include In-Plane Switching (IPS) which is a newer LCD screen technology that is supposed to be even better than the traditional. These displays feature a slim, sleek design making them compact and able to be utilized for numerous applications. LCD

displays are used in several sectors including consumer electronics, healthcare, retail, industrial environments, and the automotive industry (LinkedIn, 2024).

A light emitting diode display (LED) is a flat panel display that uses individual light-emitting diodes as pixels for images and videos. These displays are composed of multiple LEDs with a bright range to form an image or video on the display and are often used in a number of areas. With their high brightness levels, vibrant color palette, and energy efficiency; LED allows displays the opportunity to showcase wide viewing angles with superb contrast ratios making this type of display screen technology a prime candidate for diverse environments. In comparison to typical or standard display technologies, light emitting diode displays are known to perform with a higher level of longevity and durability as well as have a unique design flexibility generating curved or custom shaped screens. These types of displays are most commonly seen in monitors, TVs, and signs or billboards. With the uptick in popularity and innovation, this technology has become smaller with higher resolution and efficiency capabilities.

An organic light emitting diode display (OLED) is a flat light emitting technology composed of organic films between conductors that show light when an electric current passes through which eliminates the needs for a separate backlight which is what is generally used in regular liquid crystal displays (LCDs). The removal or lack of backlight results in a few advanced features including allowing each pixel to be able to individually emit light from itself or stay off resulting in better contrast levels as it relates to vibrant colors and true blacks. OLEDs are most used in TVs and wearable devices due to their flexibility, high contrast, and color reproduction (OLED-info, 2024). There are numerous advantages and features to this display technology, as they are thin and flexible with faster response times and more unique viewing angles when compared to other displays allowing for curved or rollable designs that may not seem plausible for other technologies. Although OLED displays are usually pricier than traditional LCDs they continue to lead in popularity thanks to their visual performance and efficiency.

A mini light emitting diode display (mini-LED) is a type of light emitting diode display that uses smaller LED lights to concentrate on more precise backlighting control with enhanced brightness and contrast. Since this display is more focused on controlling the backlight, it is easier to improve the high dynamic range performance because of the local dimming zones known as full array local dimming (Android Authority, 2024). Mini-LEDs may seem like the same technology as a traditional LED; however, they do differ in size and application as mini-LEDs are primarily responsible for backlighting LCD screens. They usually have better energy efficiency, brightness, and image quality because they can support finer gradations of brightness.

Another aspect that must be taken into consideration is the potential use of a touchscreen display rather than a traditional monitor or display. Touchscreens are electronic displays that work as an input device to enable direct interaction through the touch of a finger or stylus tool as a means to use devices such as smartphones, tablets, and laptops to access and use content. Thanks to the intuitive interface it provides touchscreens have become increasing popular in areas including consumer electronics, industrial control systems, point-of-sale terminals, and interactive kiosks; enabling seamless navigation through applications, games, and web content without the need for external input devices as once originally needed before (TechTarget, 2024).

Choosing a touchscreen display over a regular LCD display for a Raman spectrometer offers several advantages:

1. Interactivity: Touchscreens allow direct interaction with spectroscopy software and data, enhancing user control and navigation without additional input devices.

2. Ease of Use: Navigation through menus and data manipulation is more intuitive with touch-based controls, improving workflow efficiency.

3. Real-Time Adjustments: Users can make immediate parameter adjustments by tapping the screen, useful during data acquisition or experiment setup.

4. Compact Integration: Combining display and input functionalities in one unit simplifies setup and is ideal for portable spectrometer designs.

5. Enhanced Visualization: Touchscreens support interactive data exploration like zooming and swiping, providing dynamic ways to analyze spectroscopic results.

However, touchscreen displays may be costlier and require more maintenance compared to regular LCDs. The decision to use a touchscreen depends on project requirements for usability, interactivity, and integration complexity (OpenAI, 2024).

There are a variety of touch panels giving us five main options:

- Resistive touch
- Optical imaging touch
- Projected capacitive touch
- Infrared touch
- Surface acoustic wave

Each touch type offers unique benefits in terms of sensitivity, durability, and responsiveness that will be further discussed below.

Resistive touch technology works by detecting pressure placed on the screen. Two conductive coated layers are separated by a gap, when the layers touch that means pressure has been applied causing a change in electrical current from that location (TechTarget, 2024). Resistive touch's input methods include a variety of objects like a finger, gloved hand, pen or stylus tool. Pros to choosing this form of touch technology include its easy activate feature accepting basically any input, low power consumption, tactile feel of the screen, high resistance to surface contaminants and/or liquids such as oil, moisture, dirt, dust, grease as well as it being the lowest cost touch technology out of all five options (Tru-Vu Monitors, 2024). This type of technology is primarily used for point-of-sale or kiosks; an example would be signing your name with a stylus after completing a transaction. While resistive touchscreens are usually more affordable, they are less durable compared to other technologies as they do not allow for multipoint functionality and offer limited clarity.

Optical imaging touch technology works based on changes in light or reflections when touching the screen by using cameras and sensors. How it works is that cameras and sensors are within the display's perimeter and serve the purpose of analyzing the light patterns. If a finger touches the display that light pattern is disrupted triggering the sensors to calculate the exact location of the touch. This technology is ideal for interactive displays as it provides accurate detection with limited screen contact (TechTarget, 2024). Advantages of using this technology in comparison to others is there is improved accuracy thanks to the multi-touch detection functionality, greater efficiency, and accepts numerous input methods like gloved or bare fingers and stylus tools with adaptability for various environments.

Projected capacitive touch works by detecting touch through changes in capacitance. How it works is that behind the display screen is a transparent layer made up of a grid of embedded electrodes. When the electrostatic field generated by the electrodes is interrupted there is a change in capacitance signal a touch has occurred. The grid changes are then analyzed in order to accurately determine the location of the touch and movements. This technology is found in everyday devices including smartphones, tablets, GPS, and laptops making it a great option to fit in anything and for when you do not know what to choose (ViewSonic, 2024). Projected capacitive touch allows for multitouch functionality as well with high precision and responsiveness. Projected capacitive touch's advantages include its sensitivity, scratch resistance, durability, reliability, and multiple environment operation. This technology is protected via multiple options including cover glass and special coatings making them suitable and adaptable for various applications and industries.

Infrared touch technology, also known as IR touch, uses infrared light beams emitted across the surface of the display to detect and respond to touch. Applications where this type of technology can be used or found are interactive screens, public information kiosks, ATMs, and ticketing machines. When the invisible grid panel of infrared light is disrupted that means there was a touch detected, triggering the infrared sensors. The touch location is found by carefully analyzing the light beam interruption pattern. Benefits to using this form of touch technology include the ability to have touch detection of a diverse set of inputs including fingers, gloves, stylus tools, etc., resistance to surface contaminants such as dirt and dust, and increased durability. This type of touch technology supports multitouch functionality and works particularly well in harsh environments, making it suitable for industrial use. However, infrared technology performs poorly when in heat or direct sunlight as the accuracy of the screen may be affected which may limit the locations it can be used.

Surface acoustic wave touch technology, also known as SAW touch technology, uses ultrasonic waves to detect and respond to touch. The way this technology works is by using the surface of the display to transmit an invisible grid of ultrasonic waves through piezoelectric transducers and receivers that surround the edges of the screen (Tru-Vu Monitors, 2024). Touch is detected when a disruption is received by the transducers based on whatever touches the screen absorbing some of the transmitted waves. Input methods for these screens include fingers, gloved hands, and stylus tools. Benefits to this technology include superior optical clarity, high touch sensitivity, higher quality scratch resistance compared to surface or projected capacitive technology, increased visibility and durability. However, SAW touch technology does have its disadvantages. This technology is limited in its ability to protect from contaminants as they may create non-touch areas on the screen, touch activation is ineffective using non-soft items like pens or fingernails, water droplets can cause false touch detection, more prone to screen scratch unlike other touch technologies. Surface acoustic wave technology is commonly used in public transportation areas like airports and train stations as well as kiosks, museums, and shopping malls (Nelson Miller Group, 2024).

Understanding these different types of screen displays as a whole can help in choosing the most suitable display technology for our specific Raman spectroscopy application based on factors like image quality, energy efficiency, interactivity, and durability.

In conclusion, while LCD and/or touchscreen displays do not always play a pivotal role in Raman spectroscopy analysis it is a useful tool for facilitating user interaction and interpreting/displaying data. The ability to account for information

including instrument settings, spectral data, real-time monitoring, and calibration information makes it a valuable tool for Raman spectroscopy.

3.6.1 Screen Display Market Comparison

The market for screen displays is increasingly competitive and rapidly evolving, driven by innovations in display technology and increasing consumer demand for high-resolution, immersive visual experiences. Various types of display technologies such as LCD (Liquid Crystal Display), OLED (Organic Light-Emitting Diode), MicroLED, touchscreen, and e-ink are catering to a wide range of applications including smartphones, tablets, and laptops to TVs, automotive displays, and AR/VR devices. There has been an uptick in certain trends shaping the display screen market include the transition towards bezel-less designs, higher refresh rates, HDR (High Dynamic Range) support, and energy-efficient displays. Moreover, the market is witnessing a shift towards flexible and foldable display technologies, enabling novel form factors and applications in wearable devices and foldable smartphones. Some of the most popular screen display manufacturers include Samsung Display, LG Display, BOE Technology, Sharp Corporation, and Japan Display Inc which are brands known for their innovation in display quality, durability, and power efficiency. As demand grows for larger displays with better visual performance across various sectors, the display screen market is in a race for who can be the most innovative and efficient.

Based on the criteria discussed above, we narrowed down our search to three screen displays available on the market: NewHaven Display NHD-0216K1Z-FL-YBW, Waveshare 2-inch IPS LCD Module, and HAMTYSAN 8-inch Raspberry Pi Display. The features, advantages, and disadvantages of each will be disclosed and present via a table for display.

3.6.1.1 NewHaven Display NHD-0216K1Z-FL-YBW

The NewHaven Display NHD-0216K1Z-FL-YBW is a compact OLED display commonly used in electronic devices that require space efficiency and limited visual information like in small panels or electronics. For general applications, an OLED display like this can be used to show status updates, general information, or user prompts. Features included in this component include low power consumption, easy interfacing, 2-line by 16-character configuration, yellow-green backlight, compact size, 2560 x 1600 display resolution, Twisted Nematic (TN) lcd type, parallel interface, high contrast, and a wide viewing angle (Mouser Electronics, 2024). When it comes to Raman spectroscopy, this display screen can be integrated into the spectrometer to communicate vital information to users and operators. However, with this selection there is a disadvantage of both limited display size and text-based information. With a price of $9.99 being on the

smaller scale price wise of our display screen selections this display offers a compact and versatile interface but does not fully give us what we are looking for in terms of user interface capabilities and customizations.

3.6.1.2 Waveshare 2-inch IPS LCD Module

The Waveshare 2-inch IPS LCD Module display is an In-Plane Switching (IPS) compact display module using an SPI interface for communication. This display module features a 2-inch display size, 240 x 320-pixel display resolution, high resolution, SPI interface, wide compatibility, and an optional built-in touchscreen. The Waveshare LCD display is ideally used for applications that require a small yet observable display reading. Regarding Raman spectroscopy, this LCD display can serve the purpose of displaying spectroscopic data, an intuitive user interface, display data logging and analysis and allow for system status monitoring in real time. Compared to the previous LCD selection the Waveshare offers a larger display size, better backlight for low light conditions, and allows for easier integration thanks to the Serial Peripheral Interface (SPI) which is compatible with other devices. The Waveshare 2-inch IPS LCD Module display presents itself as a solid candidate for usage within a Raman spectrometer based on its compactness, versatility, display technology, and interface.

HAMTYSAN 8-inch Raspberry Pi Display

The HAMTYSAN 8-inch Raspberry Pi display is an LCD touchscreen display designed to support Raspberry Pi single-board computers. The HAMTYSAN display includes features such as an 8-inch screen size, display resolution of 1920 x 1080 pixels, high resolution, touchscreen functionality with specifically capacitive touch, Thin Film Transistor Liquid Crystal Display (TFT), fast response times, and solid color reproduction. Industrial projects, educational purposes, and gaming consoles are some of the few applications of this display model. In comparison to the previously discussed LCD display selections, the HAMTYSAN 8-inch Raspberry Pi display offers a multitude of advantages including but not limited to display size, functionality, compatibility of components, customization of user interface making it ideal for applications requiring a focus on detailed data visualization and an interactive user interface like a Raman spectrometer. This model seems to be the best candidate for our project as it offers both versatility and flexibility for the project needs as well as is compatible with our choice of microcontroller, which was the Raspberry Pi 3 Model B+.

Table 3.7.1 Display Screen Comparisons

Features	NewHaven Display	Waveshare	HAMTYSAN

Screen size	2-line by 16 characters	2 inches	8 inches
Display resolution	2560 x 1600 pixels	240 x 320 pixels	1920 x 1080 pixels
Interface	Parallel	SPI	GPIO
Display type	OLED	LCD	TFT LCD
Touchscreen capability	No	No	Yes
Type of touchscreen	-	-	Capacitive touch
Dimensions	4.9” x 1.7” x 0.4”	2.28” x 1.37” x 0.19”	8.74” x 5.98” x 2.24”
Operating Voltage	5 V	3.3 - 5 V	5 V
Compatible with Raspberry Pi 3 Model B+	Yes	Yes	Yes
Pricing	$9.99	$14.65	$65.49

3.6.1.3 Screen Display Final Selection

Based on the research conducted as shown in the table above the touchscreen display used for this project was the HAMTYSAN 8-inch Raspberry Pi display. Although this option was pricier, the benefits it provided outweighed the higher cost associated with it. In comparison to the other touchscreen display options, the one we selected has a touchscreen capability with a larger display size while still maintaining visibility and portability allowing for the showcase of detailed spectroscopy data while also including a customizable user interface, easy compatibility and installation with other components. The device is also a capacitive touch screen ensuring multitouch functionality, high sensitivity, and quick responsiveness. The advantages of superior image clarity, high scratch resistance, and surface and liquid contaminant control make it an excellent choice as it regards to the use of touchscreen display and touch technology options that are available in today’s market. In addition to the features, it is also a suitable match for the previously selected microcontroller, Raspberry Pi 3 Model

B+, we are using as the command center of our operating system allowing for a seamless setup process between components.

3.7 Analog-to-Digital Converter

In Raman spectroscopy, to receive the data from the signal emitted by photodiode to the LCD display, it must be converted from an analog to digital signal. An analog-to-digital converter (ADC), specifically the Bridgold MCP3008 in the RAID system, was an essential piece of our project and a widely used integrated circuit that converted the analog signals into digital data. Features include 8 separate input channels, Serial Peripheral Interface (SPI), and up to 1024 voltage levels. This ADC played a crucial role in bridging the gap between the analog signals from sensors, such as the photodiode (Thorlabs DET 210/M) in Raman spectroscopy, and the digital processing capabilities of the Raspberry Pi microcontroller to control energy and efficiency.

3.8 Software Research

Software has one of the most vital roles in advancing the field of Raman spectroscopy by enhancing instrument control, optimizing data acquisition, and enhancing overall usability. Within Raman spectroscopy, software is the backbone or supervisor of the system ensuring that users and researchers can successfully and efficiently operate spectroscopy machines.

Software is instrumental in controlling and facilitating the operation of certain experimental parameters including sample positioning, laser power, and wavelength selection (ThermoFisher Scientific, 2024). With this level of control there is somewhat of a guarantee for consistency and reproducible results, which is vital for gathering reliable data.

To ensure smooth integration of Raman spectroscopy with other analytical instruments and techniques, software is essential. For instance, software-controlled coupling of Raman spectroscopy with microscopy or imaging systems allows for an extensive and comprehensive sample analysis across different scales. This integration provides both spectroscopy users and researchers with a better understanding of the sample’s characteristics and behaviors, allowing for the expansion of the scope and versatility of Raman spectroscopy in scientific studies and investigations.

Additionally, software innovations and advancements contribute to simplifying instrument calibration and maintenance processes. Modern Raman spectrometers are built with software algorithms that automate calibration procedures, which can streamline the setup of instruments and reducing

complexity and time. Due to this, the efficiency of the measurements and accuracy and reliability of the Raman instruments are increased. Based on these software functionalities, researchers and industry professionals can minimize operational challenges and streamline performance of Raman instruments leading to the overall enhancement of the effectiveness of the Raman spectrometer in numerous applications.

Also, software advancements contribute significantly to instrument calibration and maintenance. Modern Raman spectrometers are equipped with intelligent software interfaces that automate calibration routines, reducing the complexity and time required for instrument setup. This not only enhances the efficiency of spectroscopic measurements but also ensures the long-term reliability and accuracy of Raman instruments in research and industrial applications.

Furthermore, software responsible for aiding in the handling data and organizing information in the context of Raman spectroscopy. There are software platforms that give researchers access to tools to effectively store, retrieve, and share spectral data. This organized approach to data management fosters transparency and reproducibility in scientific research, enabling researchers to easily archive and access spectral datasets. These capabilities are fundamental for supporting collaborative research endeavors and facilitating knowledge sharing within the scientific community. With this software, collaboration can be fostered to improve progress in scientific fields using Raman spectroscopy.

Overall, software serves as a vital foundational component in advancing Raman spectroscopy by enabling precise instrument control, facilitating integration with complementary analytical techniques, automating calibration processes, and enhancing data management capabilities (ThermoFisher Scientific, 2024). These software-driven innovations not only optimize the performance and usability of Raman spectrometers but also contribute to the overall advancement and adoption of spectroscopic techniques in various scientific disciplines. Effective use of these software tools can result in researchers and industry professionals being able to use Raman spectroscopy to address complex scientific challenges and drive innovation in the applicable fields.

In this section, we will focus on researching and selecting all required software components for this project. For a component to be selected, it must prioritize the engineering and marketing requirements stated in our house of quality and the goals for our Raman spectrometer. Several options for each component will be both evaluated and compared below discussing their pros and cons.

3.9 Coding & Technologies

The software technologies used for Raman spectroscopy are vital in terms of the collection, processing, analysis, and visualization of data. With these technologies, a non-destructive chemical analysis can be conducted thanks to a variety of programming languages, frameworks, and tools developed to fulfill the needs of Raman spectroscopy applications.

Raman spectroscopy's research applications of these software technologies are extensive as they ensure accurate analysis and characterization of molecular substances. These research applications include topics such as pharmaceuticals, biomedical applications, environmental science, security and threat detection, energy, and more (Wasatch Photonics, 2024).

Pharmaceuticals is an area in which the applications of Raman spectroscopy depend on software technologies to aid in developing and analyzing pharmaceutical drugs, testing drug purity and identification, quality control, and observe drug delivery in tissues. With the real-time monitoring and software control that is provide with Raman spectroscopy the cost and output time for new drugs is decreased with quality and consistency is maintained.

A combination of detection algorithms and spectroscopy lead to disease detection based on spectral signatures, information about interactions between macromolecules, hyperspectral medical imaging, and more in the biomedical applications of Raman spectroscopy. Based on software technologies, further spectroscopy can be pursed to visualize molecules and cells within samples.

Since Raman spectroscopy is a non-destructive chemical analysis technique, this also makes its software ideal for security and threat detection. Forensic analysis and trace sensing of biological and/or chemical agents makes for an essential application in terms of security as it is often used by the miliary, first responders, and many federal agencies including Homeland Security (Mogilevsky, 2012).

In these chemistry and chemical analyses, the coding and software technologies used allow for both quantitative and qualitative analysis of unknown substances to be conducted based on spectral matching and identification from spectral databases and chemometric models generated via these technologies. These tools for spectral simulation and quantum mechanical calculations give a more detailed look into the Raman spectra for aspects including electronic states, molecular vibrations, and intermolecular interactions.

In the case of the RAID Raman Spectrometer, it would be classified under the application categories of biomedical applications as well as security and threat

detection since the device is to be used to detect illicit or foreign substances including narcotics in drinks. The software technologies used must be able to meet our software and data analysis needs of system control, data acquisition, and spectral analysis while implementing algorithms for noise reduction, spectral processing, and system calibration.

Data processing and analysis algorithms are the heart of Raman spectroscopy software and technology. Operations such as spectral identification, baseline correction, spectral deconvolution, and more are what these algorithms oversee. Software technologies also ensure successful communication and integration between components within the Raman spectrometer and other laboratory equipment in addition to modifications of parameters and real-time monitoring.

Regarding system control and data acquisition, communication between the spectrometer and software technology are direct operating parameters like spectral range, wavelength, and integration time. In this case low-level programming languages or scripting languages are needed to interact with the hardware and develop custom software.

For spectral analysis, the raw spectral data is collected using a laser source, collected and dispersed by the spectrometer, and is then run through a software algorithm to reduce noise, calibrate the system and spectra, and normalize or correct intensity shifts.

These software technologies are what will be used to develop a user-friendly graphical interface making it easier for even non-experts to complete tasks with the Raman spectrometer such as data acquisition, data processing, and spectrum analysis. Features from this technology allow for visualization of data and components and customization of said analysis, meaning that complex tasks of chemical analysis can be performed with little to no previous knowledge of how to use the technology.

Communication protocols are an important aspect responsible for facilitating communication between the hardware side (the spectrometer) and managing data transfer and control. There are a few key aspects that must be considered.

Certain software interfaces use communication protocols to send commands and receive data to control the spectrometer. Universal Serial Bus (USB), Ethernet, or proprietary protocols are some common instrument control interfaces.

As it relates to data acquisition and transfer, with communication protocols we are to determine how data is transferred between the spectrometer and microcontroller for analysis, specifically beverage analysis in the case of RAID.

This is important for efficiently transferring spectral data for processing and analysis.

In software development, software development kits (SDKs) are often used by developers to work with communication protocols and provide high-level functions and methods to control the operation of the spectrometer and data retrieval.

To best implement communication protocols, those protocols should be within their coding environment such as Java, Python, C/C++ to organize and understand communication with the Raman instrument including command structures, data formats, and error handling. For the RAID system, we used Python programming language.

On the topic of error handling, there must be systems in place for detecting errors and recovery to continue a sustainable data transmission. Without these communication protocols one runs the risk of data corruption or loss during spectroscopy experiments.

Interoperability is defined as the level at which a software device can connect and communicate with other devices (TechTarget, 2024). Creating code that upholds the standards of communication protocols ensures compatibility with a variety of tools and instruments as it relates to software.

In terms of integration with software analysis, communication protocols also enable this. In Python, there are pre-established libraries like Matplotlib, NumPy, and SciPy to process and interpret the data received from the spectrometer through the communication protocol.

In conclusion, software technologies and communication protocols in coding for Raman spectroscopy play a key role in establishing effective communication between the hardware and software, data retrieval, spectral assessment, and management of system operations. Understanding and implementing these key components plays a critical role in developing a successful Raman spectrometer. Thanks to these technologies, Raman spectroscopy applications can maintain enhanced efficiency, accuracy, and versatility across many fields with accurate and reliable test results.

3.9.1 Software Selection

Selecting the right software for a Raman spectrometer is essential to ensure efficient data acquisition, processing, and analysis. Typically, Raman spectrometer software should offer user-friendly interfaces for instrument control,

parameter setting, and data visualization (Science Direct, 2024). Advanced features such as spectral deconvolution, baseline correction, peak identification, and quantitative analysis are also desirable for accurate interpretation of Raman spectra. Many commercial Raman spectrometers come with proprietary software tailored to their specific instruments, providing seamless integration and optimized performance. The software selected is important at every stage of Raman spectroscopy.

When choosing software for a Raman spectrometer, it's important to be mindful of compatibility with operating systems, data export capabilities, and support for additional analysis tools like chemometric models for complex sample characterization. Keeping these things in mind ensures seamless data acquisition. Instrument control over factors such as exposure time, spectral solution, and laser power to have precise setup and data collection.

Effective data processing and analysis play a role in Raman spectroscopy. Algorithms that include spectral normalization, noise reduction, peak fitting, and baseline correction should be a part of whatever software is used. Features such as these are important for improving the signal-to-noise ratio, identifying a spectral change no matter how subtle, and extracting meaningful spectral features. Moreover, the advanced statistical and chemometric tools embedded in the software help with multivariate analysis (Wiley Analytical Science, 2024). This means they make it easier to recognize patterns, classify substances, and measure the amounts of different chemicals in complex mixtures.

In addition to effective data processing and analysis, the software should provide easy-to-use visualization features to help users interpret Raman spectra. Visualization tools may include interactive overlays of spectra, labels for identifying peaks, and libraries of spectral references. User-friendly interfaces with customizable workflows simplify the analysis process, enabling users to explore spectral data efficiently and reach insightful conclusions.

Selecting the right software can also improve collaboration and knowledge sharing among research teams and institutions. Software that is compatible with multiple or common data formats and works well with other analytical software tools fosters interdisciplinary research and speeds up scientific progress. This compatibility means there is more efficiency within the research community allowing them to work faster and more progressively.

Ultimately, selecting software that meets the specific needs of the application and user preferences is crucial for maximizing the capabilities of a Raman spectrometer.

Based on the criteria discussed above, we narrowed down our search to three software technologies available on the market and compatible with our choice of microcontroller, the Raspberry Pi 3 Model B+: Java, Python, and C/C++. The features, advantages, and disadvantages of each will be disclosed and present via a table for display.

3.9.1.1 Java

Java is an object-oriented, high-level, multi-platform programming language developed in 1995 by Sun Microsystems. It is a platform independent, robust language that is secure and reliable to run operations for mobile apps to server-side technologies. Java is a language that contains the ability to large sets of data, integrate with multiple laboratory components and algorithms, and provide flexibility and scalability. Any programs written using the Java programming language are compiled using the Java Runtime Environment (JRE), to execute the programs. When it comes to Raman spectroscopy, a programming language such as this one that can handle large amounts of spectral data both efficiently and effectively is crucial in order to oversee data collection, processing, analysis, and visualization. The use of Java programming language would serve as most beneficial as it relates to higher level data analysis rather than being used at a lower level for microcontroller firmware. The libraries and frameworks in addition to cross-platform compatibility it provides make this a great tool for implementing algorithms and modifying experimental parameters.

3.9.1.2 Python

Python is another object-oriented, high-level, multi-platform programming language generally purposed and developed by the Python Software Foundation in 1991. Python programming language focuses on a wide range of applications including software development, data visualization, task automation, and more. In Raman spectroscopy, Python's extensive libraries can be used for data processing aspects like baseline correction, peak fitting, as well as statistical analysis. Compared to other programming languages Python is simpler and often referred to as easier to learn. Features that would be beneficial to spectroscopy include its flexibility, dynamic coding approach, and library components and tools. However, Python does not have its own runtime environment like Java meaning a compiler must be found that can transmit it to a host system. This is a disadvantage as it goes against the desire for the software and data analysis requirements of being a portable device with both real-time results and accuracy, which can be delayed by this. A higher-level coding language such as Python is best suited for high-level data processing within Raman spectroscopy.

3.9.1.3 C

C programming language is a low-level, general purpose computer language developed in 1972 by Dennis Ritchie of Bell Laboratories. C is a procedural language meaning it has no object or class support compared to other programming language options like Java and Python which are object-oriented programming languages (Coursera, 2023). Ideally a language like this would be used for hardware purposes or generating signal processing algorithms in Raman spectroscopy allowing for communication between hardware components and software applications. In comparison to the previously discussed programming languages, since it is a lower-level language out of the other options we selected it would be best used for programming the Raspberry Pi 3 Model B+ microcontroller firmware. C is just as powerful and effective, but complexity wise the language requires manual memory management which can increase development time, is platform dependent limiting environment accessibility, and has a minimal number of libraries available making algorithms harder or more of a challenge to implement. Although C provides both solid performance and operational control, there are significant tradeoffs between our requirements of performance, mobility, and development complexity that must be considered.

Table 3.10.1 Programming Language Comparisons

Features	Java	Python	C
Level	High	High	Low
Type	Object-oriented	Object-oriented	Procedural
Runtime environment	JRE	-	-
Communication Protocol	Transmission Control Protocol (TCP)	IPC	UART
Compatible w/ Raspberry Pi 3 Model B+	Yes	Yes	Yes

3.9.1.4 Programming Language Final Selection

For our project we ended up using the Python programming language with the Thonny IDE already installed on the Raspberry Pi 3 Model B+. Using Python

allowed us to use a programming language which operated at a high level with extensive libraries and resources that would be beneficial to and meet the needs of our spectrometer.

3.10 Analyzing the Data

Raman spectroscopy plays a critical role in a diverse number of scientific sectors due to its specifically non-destructive chemical analysis technique to provide insight into chemical structures. Data from Raman spectroscopy can shed light on analysis of molecular structures, identify substances, monitor chemical reactions, determine chemical compositions, and much more. Data analysis in Raman spectroscopy involves a mixture of integrating experimental methods, signal processing, and data interpretation to extract information regarding the sample being examined. Valuable information leading to the advancement of technological innovation, scientific research, and applications can be accrued from the data being examined.

3.10.1 Preprocessing

Before analysis, the raw spectral data collected from the Raman spectrometer undergoes preprocessing to enhance the signal quality and improve noise reduction involving baseline correction, normalization, smoothing, and wavelength calibration.

In Raman spectroscopy, baseline correction is responsible for noise reduction in the background and baseline drift. Fluorescence from an LCD display, noise of other components, or cosmic rays can interfere with the signals. Accuracy of spectral analysis is enhanced by using baseline correction to separate the Raman signals from the test sample (Bai, 2020). This step is a key component in successful interpretation and quantitative analysis of Raman spectra.

Normalization is a data processing technique that focuses on eliminating any signal intensity variations that may be caused by sample concentrations or instrument settings such as detector sensitivity and laser power. Normalization is done by dividing the data point’s intensity by a reference value that cannot be affected by any outside conditions. This process ensures that spectral trends are clear and quantitative analysis accurate by mitigating variance.

Smoothing in Raman spectroscopy is a common method to reduce high-frequency noise while maintaining the spectral features. Most used is the Savitzky-Golay (SG) algorithm which is done by placing a piece of the spectrum in a certain window of a polynomial function (Bai, 2020).

Wavelength calibration is another part of preprocessing that ensures the spectral peaks are aligned properly using the detector.

3.10.2 Spectral Analysis

After the spectra has been preprocessed, it is analyzed to gather pertinent data. There are three major aspects of this phase including peak identification, peak fitting, and chemometric analysis.

Peak identification involves selecting observable peaks to be assigned to certain vibrational modes of molecules in the sample being tested.

Peak fitting is a modeling method used to model spectral peaks using mathematical functions like Gaussian curves or Lorentzian curves to quantify intensities, positions, and widths of peaks.

Chemometric analysis is a technique used to find and pick out information from Raman spectra from the test samples (Guo, 2021). This form of analysis helps analyze complex spectral data, identify patterns and trends, and make any necessary correlations between data.

3.10.3 Interpretation

To understand Raman spectroscopy data, spectral traits must be observed and correlated with the test sample's chemical composition, physical characteristics, and molecular structure using chemical makeup, phase analysis, and quantitative analysis.

Chemical makeup or identification is composed of matching Raman bands to certain vibrational modes of molecules or functional groups. With this tool, researchers can compare the spectra data of an unknown sample to that of a sample that has already been used or referenced before.

Phase analysis in Raman spectroscopy focuses on studying and observing changes of the physical state of materials like phase transitions based on their spectral signature. This analysis provides more insight into materials and their differences based on molecular arrangements and crystal structures.

Quantitative analysis in Raman spectroscopy is calculating the concentration of compounds in a sample being tested. Estimates are made by correlating peak intensities with known standards and/or using calibration curves.

By using these steps along with the technologies and techniques, valuable knowledge from Raman spectroscopy data can be used to make strides in numerous industries within a range of applications.

3.10.4 Data Analysis using Software & Technology

As it has been stated many times before, Raman spectroscopy is a powerful analytical technique used across several scientific fields, including chemistry, materials science, and biology, among others. Using this technique, we are given insight into the composition, characteristics, and molecular structure by measuring the vibrational modes of the molecule samples being tested. However, interpretation of these spectra offers themselves as a challenge due to spectra characteristics of subtleness and overlapping bands which is why data analysis using the proper software tools and technologies plays such a crucial role in gathering vital information from the spectra data.

Software tools and technologies designed for Raman spectroscopy are important in streamlining data analysis workflows and enhancing the accuracy and efficiency of spectral interpretation.

An important analysis aspect is spectral processing, which focuses on smoothing, normalization, and baseline correction. These steps enhance clarity and reliability of the spectral features by removing noise and/or artifacts.

Software packages such as Labspec, Thermo Scientific OMNIC, and Horiba LabSpec include specific modules for spectral preprocessing, allowing for precise preprocessing regarding data.

Data analysis software plays a key role in identifying and assigning peaks, crucial for deciphering molecular structure and chemical composition. The algorithms within these tools can automatically pinpoint peaks and aid in associating them with vibrational modes or functional groups. This automated process speeds up analysis considerably and minimizes the risk of errors. Popular software systems like WiRE™ by Renishaw and GRAMS Suite by Thermo Fisher Scientific are great tools for peak analysis, providing user-friendly interfaces that enhance spectral interpretation (GRAMS Suite, 2024).
Another important area to consider is multivariate analysis, which allows for a more comprehensive understanding of complex Raman datasets. Techniques such as principal component analysis (PCA) and hierarchical clustering are used to recognize underlying patterns and connections within spectral data (SpringerOpen, 2024). These approaches are valuable for distinguishing between various sample groups, identifying unusual data points, and revealing nuanced differences that might not be obvious through visual examination alone. Specialized software platforms like The Unscrambler® X and TIBCO Spotfire provide advanced multivariate analysis tools specifically designed for Raman

spectroscopy applications. These tools are aimed at helping researchers extract deeper insights and make sense of intricate spectroscopic data more effectively.

Connecting data analysis software with spectral databases improves the dependability and precision of interpreting spectra. These databases hold a large collection of reference spectra that can assist in identifying unfamiliar compounds, verifying known substances and tracking compound characteristics. Tools such as KnowItAll Informatics System Software and SpectraGryph optical spectroscopy software provide access to these databases, so researchers can access extensive reference libraries for more thorough data analysis (Wiley Science Solutions, 2024).

Several main software tools and technologies that facilitate Raman spectroscopy data analysis:

- Commercial Software Packages: Examples include Labspec, OMNIC, and GRAMS/AI, which offer user-friendly interfaces for preprocessing, analysis, and visualization of Raman spectra.
- Open-Source Software: Options like RamanAnalysis, RamanPy, and PLS Toolbox provide tools for spectral processing, chemometric analysis, and data visualization.
- Python Libraries: Libraries such as SciPy, NumPy, and scikit-learn are commonly used for custom analysis and scripting.
- Matlab: Often used for advanced spectral analysis, chemometrics, and data visualization. (OpenAI, 2024)

In conclusion, the application of set software tools and technology for Raman spectroscopy data analysis grants researchers the capacity to maximize the use of spectral data. By using these tools, the accuracy and reliability of spectral information is increased allowing for further advancements in the research and development industries of multiple scientific fields. As technology continues to evolve, the future of Raman spectroscopy is set to further innovate and change the way researchers harness spectral data for scientific discovery.

3.11 Hardware Research

This section will concentrate on researching and selecting all required hardware components for the project. For a component to be selected, it will need to prioritize our engineering and marketing requirements outlined in our house of quality and our goals and objectives for our Raman Spectrometer. We will evaluate and compare several options for each component, emphasizing their pros and cons.

3.11.1 Power Source

Our Raman Spectrometer will be powered to function as intended. The rotating stage is not manual therefore it will need to have a power source. Said power source will need to also serve as the power source for the microcontroller, the light source, and the camera. There are multiple ways to power a spectrometer: battery power, solar power, power over ethernet, and AC/DC power. Due to our constraints and requirements, we will limit our focus to battery power and AC power.

3.11.2 Battery Power

Battery power offers portability, making it ideal for fieldwork or applications where a constant power source is unavailable. Rechargeable batteries, such as lithium-ion or nickel-metal hydride, can be used to minimize ongoing costs. However, the capacity of the batteries and the power consumption of the spectrometer must be carefully balanced to ensure sufficient operating time between charges or battery replacements. Additionally, the weight and size of the batteries can affect the portability of the spectrometer.

3.11.3 AC Power Adapter

Using an AC power adapter provides a reliable and constant power source, making it suitable for stationary spectrometer setups in laboratories or industrial settings. The adapter converts AC voltage from a wall outlet to the DC voltage required by the spectrometer. This method eliminates the need for battery replacements or recharging and reduces maintenance costs and downtime. However, the spectrometer must be located near an AC power source; this requirement limits its mobility. Additionally, power quality issues such as voltage fluctuations or electrical noise in the AC supply can affect the spectrometer's performance. This is why proper power conditioning may be necessary.

In Table 3.12.1, we compare the power supplies. The AC power adapter was chosen since it met our requirements. Our Raman is designed to be stationary so a battery-operated version would only add unnecessary maintenance.

Table 3.12.1 Power Supply Selection

Feature	Wall adapter	Battery Power
Portable	No	Yes
Long run cost-effective	Yes	No
Easy to use	Yes	Yes

Environmentally friendly	Yes	No

4 Standards and Design Constraints

This section of the paper presents a detailed overview of the current standards and calibration methods used in Raman spectroscopy to ensure accurate and precise measurements. Given the critical role of Raman spectroscopy in drug safety and efficacy, establishing, and adhering to stringent standards is paramount.

4.1 ASTM International Standard E1683

To ensure the accuracy and reliability of Raman measurements for drug analysis, proper calibration and validation procedures are essential. Reference materials with well-defined Raman spectra are used to calibrate the instrument's wavenumber scale and intensity response. These standards are often pure active pharmaceutical ingredients (APIs) or well-characterized mixtures. The American Society for Testing and Materials (ASTM) International standard E1683, "Standard Practice for Testing the performance of Scanning Raman Spectrometers," originally published in 2002, with a revised edition released in 2022, provides general guidelines for calibrating Raman instruments, although it predates some modern technologies.

The E1683 standard emphasizes the importance of regularly testing a Raman spectrometer to monitor its performance. This helps identify potential issues like degradation in sensitivity, resolution, or wavelength accuracy before they significantly impact data quality (ASTM International, 2022). This standard also outlines procedures for evaluating various performance metrics, including wavenumber accuracy, spectral resolution, and SNR. This test ensures the instrument accurately assigns wavenumbers (inverse wavelengths) to Raman peaks; standard reference materials with well-defined Raman shifts are used for calibration (ASTM International, 2022). This standard also provides methods to assess resolution, referring to the instrument's ability to distinguish between closely spaced Raman peaks, using reference materials with narrow peaks (ASTM International, 2022). High SNR indicates a clear signal compared to background noise, crucial for obtaining reliable data. E1683 suggests methods to evaluate SNR using reference materials with strong Raman scattering. By using these tests, timely maintenance, or repair to maintain optimal performance is ensured (ASTM International, 2022). While E168 serves as a valuable starting point, it is important to acknowledge its limitations. The standard primarily focuses on general performance testing and doesn't delve into specific considerations for different Raman applications, such as drug analysis. Additionally, the standard predates some advantages in Raman technology, and

users may need to adapt the procedures for newer instruments with different functionalities. In conclusion, ASTM E1683 remains a widely used standard for evaluating the performance of scanning Raman spectrometers. By following its guidelines, researchers and quality control personnel can ensure the instrument is functioning optimally, leading to reliable and consistent Raman data for various applications, including drug analysis. However, it is crucial to recognize the standard's limitation and potentially supplement it with additional application-specific testing procedures for comprehensive Raman data quality assurance.

4.2 ASTM International Standard E1840-96(2020)

The ASTM International standard E1840-96(2020), titled "Standard Guide for Raman Shift Standards for Spectrometer Calibration," serves as a valuable resource for researchers and analysts seeking reliable Raman data (ASTM International, 2020). This standard guide does not delve into the specific procedures for calibrating Raman spectrometers. Instead, it focuses on providing a compilation of Raman shift values for readily available common liquid and solid chemicals (ASTM International, 2020). These well-defined Raman shifts can be used as reference points to calibrate the wavenumber scale of a Raman spectrometer. The key aspects of ASTM E1840-96(2020) include reference materials, selection criteria, and data acquisition practices. The guide offers a table listing Raman shift values for eight commonly used reference materials, including silicon (Si), cyclohexane (C6H12), and diamond (C) (ASTM International, 2020). These materials are chosen for their well-characterized Raman spectra with sharp, intense peaks. The inclusion of a particular material in the standard guide hinges on several factors. The material should be readily available, exhibit strong Raman scattering, and possess well-defined, non-overlapping Raman peaks across a broad spectral range (ASTM International, 2020). While the guide does not specify calibration procedures, it emphasizes the importance of adhering to good laboratory practices (GLP) during Raman spectral acquisition. This includes factors like laser power selection, integration times, and baseline corrections (ASTM International, 2020). ASTM E1840-96(2020) plays a crucial role in ensuring the accuracy and reliability of Raman spectroscopic data. By utilizing the reference Raman shift values provided in the standard, researchers can calibrate their instruments to ensure accurate wavenumber assignments for the observed Raman peaks. This enables proper identification and analysis of target molecules. Additionally, the ease of access and availability of the listed reference materials make this standard guide a practical tool for routine Raman analysis in various fields.

It is important to acknowledge the limitations of ASTM E1840-96(2020). The standard primarily focuses on commonly used reference materials and might not encompass all potential Raman applications. Researchers working with less common materials might need to consult additional resources or establish their own reference standards. Furthermore, the standard predates spectral variations

based on instrument specifics. In conclusion, ASTM E1840-96(2020) stands as a valuable resource for ensuring accurate and reliable Raman spectroscopic data. By providing a readily accessible set of reference Raman shift values for common materials, this standard guide facilitates instrument calibration and promotes consistent data interpretation across various research and analytical settings. However, it is crucial to acknowledge the standard's limitations and potentially supplement it with additional application-specific reference materials and protocols for comprehensive Raman data quality assurance.

4.3 Validation

Once calibrated, the Raman system's performance for a specific drug analysis application needs to be validated. This involves analyzing standard samples with known compositions and comparing the obtained Raman spectra to established reference spectra or data from other validated analytical techniques. Statistical methods are employed to assess factors like accuracy, precision, linearity, and limit of detection.

Unfortunately, there is a current lack of widely accepted, comprehensive standards for using Raman spectroscopy specifically for drug analysis within major pharmacopeias like USP (United States Pharmacopeia) or Ph. Eur. (European Pharmacopoeia). Despite this, researchers are actively developing and validating Raman-based methods for specific drugs and application; this paves the way for future inclusion of standardized Raman methods in pharmacopeias.
Realistic Design Constraints

Economic and Time Constraints

As college students working on the RAID project, we confront substantial financial constraints that influence our approach to resource acquisition and project development. With limited financial resources, we must carefully plan our spending and make strategic selections about which components and materials to invest in. High-end or specialized equipment may be financially prohibitively expensive, forcing us to consider alternate options or innovative workarounds to meet our project objectives within budgetary limits. Furthermore, we must consider continuing operational expenditures such as maintenance, calibration, and consumables, which can quickly pile up and stretch our restricted budget. Balancing the demand for quality and performance with cost-effectiveness is an ongoing challenge that requires careful budget management and resource optimization.

In addition to financial constraints, time constraints are a major impediment to the RAID project's success. As college students with academic obligations and limited project schedules, we must work efficiently and effectively to meet our objectives within the time constraints. With only two semesters to complete the

project, time management is critical, forcing us to prioritize work, set realistic deadlines, and distribute resources appropriately to maximize productivity and development. The pressure to reach project goals and deliverables on time can be strong, needing excellent team communication, coordination, and teamwork to ensure successful project execution.

Furthermore, the time constraints of the academic calendar limit the size and complexity of the RAID project. We must carefully scope our project objectives and deliverables to fit within the available time frame, avoiding overly ambitious or unrealistic aims that could cause project delays or failure to achieve deadlines. This necessitates a disciplined approach to project planning and execution, emphasizing producing significant results within our academic schedule. Despite these hurdles, time constraints can act as a catalyst for creativity and innovation, motivating us to streamline procedures, prioritize critical tasks, and make smart decisions to maximize project outputs within the timeframe provided.

When compared to the competitors of the RAID project, the involvement of these large companies' product owners greatly reduces financial limitations that would otherwise hamper project completion. Unlike college students, the companies' access to financial resources, such as loans and investments from investors, gives it a significant edge in raising funding to support their Raman spectrometers' development. With increased financial stability and access to money, these companies may invest in high-end equipment, specialty components, and experienced personnel without having to worry about budget constraints. This allows the project team to pursue ambitious goals, investigate novel solutions, and optimize project outcomes to a larger extent than would be possible with little funding.

However, despite the companies' financial benefits, time is still a significant limitation that must be carefully controlled. The companies' ability to sustain their project developments over time is determined by its profitability and financial sustainability. Depending on the companies' financial reserves and investment strategy, there may be pressure to provide results within a specific timeline to justify ongoing investment and support. This time limitation creates a sense of urgency for their projects, necessitating efficient project management, effective decision-making, and timely execution to fulfill project milestones and objectives. Failure to make timely progress and provide real results risks jeopardizing the funding and viability of their projects, emphasizing the need of matching financial resources with project timetables and deliverables.

In conclusion, while the engagement of a large corporation offers substantial benefits in terms of financial resources and support, time remains a critical constraint that must be carefully handled. By utilizing their financial stability and access to cash, the corporation can overcome many of the financial barriers that college students have. However, the pressure to provide results within a specific

timeline emphasizes the significance of effective project management and strategic decision-making to assure project success and long-term viability. As college students working on the project, we face fiscal constraints that limit our resource allocation and project scope. Limited financial resources force us to prioritize expenditure and seek cost-effective solutions, while the academic calendar imposes stringent time constraints, pushing us to work efficiently and effectively to meet our objectives within the allocated term. Despite these obstacles, both teams must use creativity, perseverance, and strategic planning to optimize the project's effect and success.

Environmental, Social, and Political Constraints

In terms of environmental restrictions, the RAID project must ensure the endurance and reliability of the spectrometer system, especially if it is used in outdoor bar settings. Harsh environmental conditions such as rain, humidity, and temperature variations can all harm sensitive equipment and impair its effectiveness. To reduce this risk, the RAID project must emphasize the design and installation of an enclosed, weather-resistant system capable of enduring external settings while maintaining optimal operation. Similarly, competitors working on handheld spectrometers for law enforcement have similar environmental concerns, as their equipment may be utilized outdoors during field operations. Enclosures and protective casings are critical for protecting equipment from environmental threats while also assuring its efficacy and endurance across a wide range of working situations.

From a sociological standpoint, the RAID project faces the issue of introducing a new technology into a market that may be unfamiliar or uncomfortable with its ramifications. Bar owners and patrons may be concerned about the existence of a spectrometer designed to detect drugs in their facilities, thinking that it may indicate an increased danger of drink tampering or jeopardize the culture of trust and enjoyment. Furthermore, inadequate scientific literacy among bar owners and customers may create communication difficulties and opposition to utilizing the technology. To address these societal obstacles, the RAID project must focus education and outreach initiatives to demystify the technology, foster trust, and highlight the benefits of incorporating the spectrometer system inside bars.

Politically, the RAID project faces regulatory hurdles and governmental constraints that impact its scope and objectives. Initially, our intention was to develop a spectrometer capable of detecting gamma-hydroxybutyrate (GHB), a notorious date rape drug, within bar settings. However, stringent regulations imposed by the Drug Enforcement Administration (DEA) complicated our plans. In order to proceed with testing for GHB, we would have needed a licensed professor who was authorized by the DEA to handle illicit drugs. This individual would then be required to undergo a thorough vetting process, including an in-person interview with the DEA to justify the use of controlled substances for

research purposes. Also, extensive paperwork would need to be submitted, followed by at least three months' waiting period for approval, as advised by Environmental Health and Safety (EHS) at UCF. Unfortunately, this timeline was incompatible with the project's timeframe, as we were tasked with completing the project within two semesters.

Because of these political restraints, we were forced to change our strategy and focus on an alternate material for detection. After considerable deliberation, we decided to use gamma-aminobutyric acid (GABA) rather than GHB. GABA is a legal and accessible precursor to GHB, making it a suitable alternative for our spectroscopic research within regulatory constraints. While this change required a revision in our project's objectives, it enabled us to better negotiate the difficult regulatory landscape and complete our research on schedule. Our competitors in the development of handheld Raman spectrometers for the detection of illicit narcotics benefit from longer timeframes and existing agreements with governments. This enables them to handle political considerations about law enforcement techniques, civil liberties, and public views more easily. Collaboration with government agencies and stakeholders can help them set clear rules and protocols for the ethical and responsible use of their technology, reducing political risks and creating trust and responsibility in its deployment.

Despite the hurdles caused by political restraints, our proactive engagement with regulatory agencies and respect for legal rules allowed us to adapt and move forward with the RAID project. By focusing on compliance and ethical considerations, we want to negotiate political complexities while working toward our goal of establishing a dependable and effective spectrometer to improve safety and security in bar situations.

Ethical limitations are important in the development and deployment of the RAID project, especially when it comes to the use of surveillance equipment in public venues like bars. One ethical problem is individual private rights and the potential intrusion caused by the spectrometer's detecting capabilities. Bar guests have a fair expectation of privacy when socializing in public places, therefore the use of surveillance technologies must be calibrated with respect for their autonomy and personal space. Concerns have also been raised about the possible stigmatization of individuals and groups as a result of drug-detection technology, which may perpetuate stereotypes and biases. To meet these ethical limits, the RAID project must stress transparency, consent, and accountability in its execution, ensuring that the spectrometer is used in accordance with values of fairness, respect, and social responsibility.

In contrast, firms producing handheld Raman spectrometers for law enforcement face comparable ethical concerns, albeit in a different setting. The use of surveillance technologies by law enforcement authorities raises concerns about civil liberties, due process, and the possibility of abuse or misuse of authority.

Ethical restrictions include protecting individuals' rights from unwanted searches and seizures, providing fair and impartial justice, and reducing the likelihood of discriminating acts. To address these concerns, corporations must follow the legal and ethical principles that govern law enforcement actions, promote accountability and openness in technology deployment, and participate in communication with stakeholders to address community concerns and maintain public trust.

Health constraints impact the RAID project, particularly the possible health hazards related to drug use and pollution in bar environments. The spectrometer's detection capabilities may reveal residues of unlawful chemicals that pose health risks to customers, such as GHB or other hazardous drugs. To mitigate these health hazards, suitable safety precautions must be implemented, such as frequent equipment maintenance, calibration, and hygiene practices to minimize cross-contamination and assure accurate results. Furthermore, there may be worries regarding the psychological impact of drug-detection equipment on patrons' mental health, especially if it develops a culture of fear or mistrust. To address these health concerns, the RAID project must emphasize bar guests' safety and well-being while also achieving its goals of improving security and minimizing drug-related harm.

Similarly, our competitors designing handheld Raman spectrometers for law enforcement must address the health concerns connected with exposure to hazardous compounds while conducting field operations. Law enforcement officers may come into contact with harmful narcotics, chemicals, or unknown substances that, if handled or identified incorrectly, offer immediate health risks. To reduce these hazards, businesses must provide extensive training, safety equipment, and procedures for handling and disposing of hazardous chemicals. Furthermore, there may be worries about the long-term health consequences of frequent exposure to potentially hazardous chemicals, necessitating continued monitoring and assistance for drug detection and enforcement professionals. Overall, overcoming health limits necessitates a proactive approach to risk management, training, and assuring the well-being of those impacted by Raman spectrometer technology.

Manufacturability and Sustainability Constraints

Manufacturing and sustainability restrictions are important issues for the RAID project, especially when it comes to the spectrometer system's production and environmental impact. One facet of manufacturability is to ensure that the spectrometer components are designed and assembled in an efficient and scalable manner. The RAID project seeks to expedite the manufacturing process and enable system replication for mass production by providing a 3D CAD model for the housing and full assembly instructions. This technique enables for better customization and adaptation to various industrial conditions, resulting in more efficient production while keeping uniform quality standards.

Furthermore, the RAID project prioritizes sustainability, aiming to reduce its environmental impact and promote responsible resource usage throughout the product's lifecycle. The project's goal is to reduce waste and energy consumption related to manufacture and disposal by incorporating durable and recyclable materials into the spectrometer housing. Furthermore, the availability of CAD models and instructions allows customers to personalize and improve their spectrometer cases, increasing the product's lifespan and minimizing the need for frequent replacements. This emphasis on sustainability is consistent with broader initiatives to encourage eco-friendly activities and reduce the environmental impact of technology development and use.

Competitors creating handheld Raman spectrometers for law enforcement may confront comparable manufacturability issues, but with different sustainability constraints. To maintain dependability and performance under challenging field settings, portable device manufacturers must carefully consider design optimization, material selection, and assembly procedures. However, the emphasis on sustainability may differ according to the company's aims and target markets. While some organizations stress sturdiness and longevity to reduce product turnover and waste, others focus on lightweight and compact designs to improve portability and consumer convenience. Overall, resolving manufacturability and sustainability limits necessitates a comprehensive approach that considers both technical and environmental considerations to ensure the product's long-term viability and success.

In addition, companies creating handheld Raman spectrometers may encounter specific obstacles in terms of regulatory compliance and certification requirements, which can have an impact on the product's manufacturability and sustainability. Compliance with industry standards and government regulations is critical for market access and customer confidence, but it may increase the complexity and cost of the production process. Companies that address these difficulties proactively and invest in comprehensive quality assurance and certification systems can improve their product's manufacturability and sustainability while retaining regulatory compliance and market competitiveness. Lastly, maintaining proprietary control over product information, particularly in terms of spectrometer construction, provides a manufacturing limitation.

Light Budget Constraints

Light budget limits provide a serious barrier for the RAID project, as the system can only use one laser source (with a maximum power of 500mW). This limitation restricts the quantity of light that can flow through the system and interact with the sample, resulting in a reduced signal captured by the spectrometer. As a result, the spectrometer's detection sensitivity and overall performance may be degraded due to the limited light budget, demanding careful tuning of optical

components and signal processing algorithms to improve signal-to-noise ratio and ensure trustworthy readings.

In contrast, competitors building handheld Raman spectrometers confront different light budget limits, particularly those intended for outdoor use. The need to obtain an adequate Raman signal outdoors, where ambient light levels may be higher and sample distances vary, necessitates measures to improve the device's light budget. These competitors' methods include the use of numerous lasers in their spectrometer architecture. By using two lasers instead of one, they may enhance the quantity of light available for Raman excitation, improving signal intensity and detection sensitivity under difficult outdoor conditions.

While using numerous lasers may help competitors overcome some of their light budget limits, it also adds complexity and cost to the spectrometer's design and operation. Managing power consumption, thermal management, and laser alignment becomes more difficult when there are several laser sources, thereby compromising the device's portability, reliability, and overall performance. Furthermore, the necessity for additional laser sources may increase the spectrometer's size, weight, and cost, limiting its usefulness and accessibility for specific applications or users.

Overall, while the RAID project has light budget limits due to a single laser source, competitors creating handheld Raman spectrometers have unique issues linked with outdoor use and the requirement for higher light budget. Understanding and resolving these limits allows the RAID project and its rivals to optimize the performance and utility of their spectrometer systems for varied applications and environments.

4.3.1 ICH

These efforts often leverage existing compendial methods for identification and purity testing, adapting them to a Raman spectroscopy framework. The International Council for Harmonisation (ICH) guidelines provide a framework for developing and validating analytical procedures for pharmaceuticals (ICH, 2023). These guidelines, while not specific to Raman spectroscopy, offer principles that can be adapted for Raman-based drug analysis methods. For instance, the ICH Q2 (R1) guideline on validation of Analytical Procedures emphasizes the importance of demonstrating factors like accuracy, precision, specificity, limit of detection, and linearity (ICH, 2005). Building upon existing general standards, a robust validation process for Raman systems used in drug analysis should consider the specific drug and application specificity, accuracy and precision, limit of detection (LOD) and limit of quantification (LOQ), linearity, and robustness. The Raman method must demonstrate that it can distinguish the target drug from potential interferences like excipients, degradation of products, or other co-formulated drugs. One should also evaluate the method’s ability to quantitatively determine the amount of the drug present with acceptable levels of

accuracy and precision. The method should be able to determine the lowest concentration of the drug that can be reliable detected or quantified. One should establish the linear relationship between the Raman signal intensity and the drug's concentration. The validation process should be thoroughly documented, including details of the instrument, reference materials, and the validation procedures employed. Additionally, regular monitoring of the Raman system's performance using reference materials is crucial to ensure consistent data quality over time. While comprehensive, drug-specific Raman validation standards are still under development, existing general standards and best practices provide a solid foundation for building reliable and robust Raman-based analytical methods for the pharmaceutical industry. By adopting these validation strategies alongside ongoing efforts to establish standardized Raman methods in pharmacopeias, researchers can ensure the reliable and consistent application of Raman spectroscopy for drug analysis.

4.4 Component Standards

The performance and reliability of Raman spectroscopy data are also influenced by the instrument's quality. This section reviews the standards and guidelines applicable to the crucial components of Raman spectrometers, including lasers, optics, filters, gratings, detectors, and sample holders. By understanding and adhering to these standards, manufacturers and users can ensure the high quality and reliability of spectroscopic measurements.

The precision and accuracy of Raman spectroscopy significantly depends on the performance of the spectrometer's components. Standards and guidelines play a crucial role in ensuring the quality and reliability of these components, thereby guaranteeing the validity of spectroscopic data. Manufacturers and users must remain cognizant of these standards to maintain the integrity of Raman spectroscopy as a critical analytical tool.

4.4.1 Laser Standards for Raman Spectrometers

The laser source is fundamental to Raman spectroscopy, providing the excitation light that induces Raman scattering. While there are not specific standards solely focused on lasers for Raman spectrometers, several factors are governed by regulations for laser safety and performance. The International Electrotechnical Commission (IEC) standard IEC 60825-1, titled “Safety of laser products – Part 1: Equipment classification, requirements, and tests,” classifies lasers based on their potential for causing harm (International Electrotechnical Commission, 2020). Raman spectrometers typically utilize Class 3B or Class 4 lasers, requiring specific safety measures like proper labeling, enclosure design, and operator training to minimize risks (International Electrotechnical Commission, 2020).

While not standards, there are important factors to consider regarding laser performance for optimal Raman results. The laser wavelength used in Raman spectroscopy influences the Raman scattering intensity. Choosing an excitation wavelength in resonance with the target molecule's electronic transitions can significantly enhance the Raman signal (Smith & Dent, 2005). The laser power must be sufficient to generate a detectable Raman signal while avoiding sample damage due to excessive heating. Optimizing laser power often involves balancing these two factors (Smith & Dent, 2005). Ideally, the laser source should be a single, pure wavelength to minimize background noise in the Raman spectrum. However, some Raman systems utilize diode lasers with broader emission profiles, requiring careful consideration of spectral filtering techniques (Smith & Dent, 2005). While dedicated standards for lasers used in Raman spectroscopy are not yet established, adhering to laser safety regulations such as IEC 60825-1 is crucial. Additionally, focusing on factors like wavelength, power, and spectral purity optimizes laser performance for generating high-quality Raman data. As Raman spectroscopy continues to evolve, the development of more specific laser standards might emerge in the future.

4.4.2 Optics Standards

Optics, including lenses and mirrors, guide the excitation light to the sample and collect the scattered light. The quality of materials and coatings, along with the precision in alignment, are crucial for minimizing losses and ensuring efficient signal collection. Optical components are made from various materials, each selected for its transparency at specific wavelengths, resistance to laser damage, and other optical properties. High-purity, low-absorption materials are preferred to minimize signal loss and avoid introducing signals into the Raman spectrum. For instance, fused silica is commonly used for UV and visible wavelengths due to its high transmission and low fluorescence. The coating applied to these optical components is equally crucial. Anti-reflective coatings are often used to enhance the transmission of light through lenses and the reflection from mirrors. These coatings are designed to minimize losses at specific wavelengths and must adhere to standards ensuring their durability, adherence, and performance over the intended wavelength range. The efficiency and longevity of these coatings are critical, especially in applications involving high-intensity laser sources. The precise alignment of optical components is vital for optimizing the optical path, focusing the laser beam accurately on the sample, and efficiently collecting the scattered light. Misalignment can lead to significant signal loss, reduced resolution, and compromised data quality. Although specific standards for alignment accuracy per se might not exist, general guidelines and best practices within the industry emphasize the importance of regular maintenance checks and calibration procedures to ensure alignment remains within acceptable tolerances. These practices are often detailed in the spectrometer's operating manual and supported by training provided by manufacturers. In conclusion, the performance of optical components in Raman spectrometers is critical for achieving high-quality spectral data. Adherence to standards and guidelines related to

material quality, coatings, alignment, and filter efficiency ensures that these components perform optimally, thereby enhancing the reliability and accuracy of Raman spectroscopic analysis.

Optical filters, including notch and edge filters, play a critical role in Raman spectroscopy by rejecting the Rayleigh scattered light while transmitting the Raman scattered light. The efficiency of these filters directly impacts the quality of the Raman signal, requiring high rejection rates of the laser line and high transmission rates for the Raman-shifted light. Standards related to optical filters focus on their spectral performance, including the bandwidth of rejection (for notch filters) or the cut-on wavelength (for edge filters), as well as their out-of-band transmission and durability under continuous laser illumination.

The grating disperses the Raman-scattered light into its constituent wavelengths. The groove density and quality of the grating directly affect the spectrometer's spectral resolution and efficiency.

4.5 List of Known Constraints

In the development of a Raman spectrometer, several critical constraints must be considered to ensure the functionality, safety, and effectiveness of the final instrument. This section outlines the key limitations and challenges faced during the design and assembly process, providing insights into the trade-offs and considerations necessary for the successful implementation of a Raman spectroscopy system.

1. **Safety Concerns with Laser Usage:** The utilization of high-power lasers as the excitation source in Raman spectroscopy presents significant safety hazards, including the risk of severe eye injuries. Ensuring safe operation involves implementing rigorous safety measures, such as proper enclosures, safety goggles, and adherence to established laser safety standards.

2. **Budgetary Limitations:** The acquisition of high-quality optical components, detectors, and other necessary equipment often involves substantial financial investment. Budget constraints may necessitate compromises in the selection of components, potentially affecting the spectrometer's performance and resolution capabilities.

3. **Optical Alignment and Stability:** The precision alignment of optical components is crucial for optimal light collection and signal detection. Misalignment can lead to reduced signal-to-noise ratios and diminished sensitivity. Additionally, the system's thermal stability impacts measurement accuracy, necessitating measures to mitigate temperature-related fluctuations.

4. **Fluorescence Interference:** Fluorescence from the sample when excited by the laser can obscure Raman signals. Selecting an appropriate laser

wavelength and implementing optical filtering or spectral processing techniques are necessary to minimize this background interference, adding complexity to the system design.

5. **Spectral Resolution and Range Considerations:** Achieving high spectral resolution requires careful selection of the dispersive element and slit width, with a trade-off between resolution and signal intensity. High-resolution configurations may compromise system throughput. The spectrometer's spectral range is determined by the grating selection, detector sensitivity, and optical filters, with extensions to the range requiring compromises in other performance areas such as resolution or sensitivity.

6. **Detector Sensitivity and Noise:** The spectrometer's performance is significantly influenced by the detector's sensitivity and noise characteristics. Implementing cooling mechanisms for the detector can enhance performance but increases the system’s complexity and cost.

7. **Light Collection Efficiency:** The efficiency of scattered light collection depends on the collection optics' design. Balancing the numerical aperture of the collection optics with the desired spatial resolution and collection efficiency presents a considerable challenge.

8. **Software and Data Analysis Requirements:** Developing or procuring software for system control, data acquisition, and spectral analysis is a non-trivial challenge that includes implementing algorithms for noise reduction, spectral processing, and system calibration.

9. **Calibration and Validation:** Accurate and reliable Raman measurements require regular system calibration using known standards, a process that can be challenging due to the availability of these standards and the calibration procedure itself.

10. **Regulatory and Standards Compliance:** Ensuring compliance with industry or research standards for measurement accuracy, repeatability, and documentation can pose significant challenges, particularly for custom-built systems intended for specific applications.

Addressing these constraints involves a complex balance of trade-offs, where improvements in one aspect of the system’s design or performance may negatively impact another. Through careful planning, innovative design solutions, and strategic decision-making, it is possible to navigate these challenges and develop a Raman spectrometer that meets the desired specifications and application requirements.

4.6 List of Requirements and Specifications

In Table 2.5.1 the specifications have been derived from current products previously talked about.

Table 4.6.1 Requirements and Specifications for Components

Component	Parameter	Specification
Laser	Laser power	80-200 mW
	Laser wavelength	532 nm
	Beam diameter	2mm
Diffraction grating	Groove density	1200 lines/mm
	Blazed	500nm
Longpass filter	Rejection wavelength	<534 nm
	Transmission	≥ 91%
Dichroic mirror	Cut-on wavelength	~532 nm
	Reflection wavelength	532nm
	Transmission	90% (average)pc
Rotation stage	Steps	360
Touchscreen	Size	56mm x 85mm x 4mm
Lens 1	Focal length	38mm
	Diameter	12.7mm
Lens 2	Focal length	25mm
	Diameter	12.7mm
Lens 3	Focal length	250mm
	Diameter	25.4mm

Lens 4	Focal length	50mm
	Diameter	25.4mm
Photodiode	Active Area	3mm

Table 4.6.2 Requirements and Specifications for RAID System

Specifications	
Total bootup time	2 minutes
Spectral resolution	< 1 nm
Total runtime	~20sec
Spectral range	540nm-790nm
Lowest concentration measured	750 mg
Computer interface	Touch screen
Touchscreen responsivity	5 ms

5 Comparison of ChatGPT and Google Gemini

ChatGPT, developed by OpenAI, and Google Gemini are two advanced AI-powered tools that significantly aid in the process of writing academic papers, essays, and research documents. Both tools have unique features that make them valuable for students, researchers, and writers looking to enhance their writing process, improve the quality of their work, and streamline their research. While both platforms offer unique advantages, they also present certain limitations that can impact their effectiveness in an educational setting. This section aims to compare the limitations, pros, and cons of ChatGPT and Google Gemini, providing practical examples from a Senior Design course perspective.

5.1 Limitations of ChatGPT and Google Gemini

One limitation of ChatGPT is its data recency; ChatGPT's knowledge is limited to its last training data cut-off, restricting access to the latest research

developments or current events, which can be crucial for a Senior Design project. Another limitation is the risk for misinformation. Despite its sophisticated algorithms, ChatGPT may occasionally generate incorrect or misleading information. Therefore, one must cross-verify information with reliable sources.

A limitation of Google Gemini is its complex query requirement. Efficient use of Google Gemini requires precisely formulated queries, which can be challenging for users unfamiliar with advanced search techniques. Google Gemini also relies heavily on internet content. This reliance on available online content can lead to biases or gaps in information, especially for niche or emerging topics not widely covered online.

5.2 Pros and Cons

5.2.1 Pros of ChatGPT:

- **Idea Generation:** ChatGPT can help brainstorm ideas, suggest research topics, and even help narrow down a broad topic to a more focused thesis statement.

- **Outline Creation:** It can assist in creating detailed outlines for papers, helping structure the document effectively from introduction to conclusion.

- **Drafting Content:** ChatGPT can generate paragraphs based on prompts or expand on bullet points, providing a solid foundation or a fresh perspective on the topic.

- **Citation and Reference Suggestions:** While it may not access the internet or the latest articles, ChatGPT can guide on how to cite sources properly and even suggest potential sources based on its training data.

- **Editing and Proofreading:** It can help identify grammatical errors, awkward phrasing, and improve the overall clarity and flow of the writing.

- **Answering Subject Matter Questions:** ChatGPT can provide explanations on a wide range of topics, aiding in understanding complex subjects.

5.2.2 Pros of Google Gemini

- **Advanced Search Capabilities**: Google Gemini can help find relevant academic papers, articles, and books with more precision, using natural language processing to understand complex queries.

- **Summarization of Sources**: It can summarize long texts, making it easier to sift through vast amounts of information and extract pertinent data without reading entire documents.

- **Trend Analysis**: For topics requiring understanding of trends and developments, Google Gemini can analyze and present the evolution of a topic over time, highlighting key milestones and current perspectives.

- **Data Visualization**: It can assist in creating charts, graphs, and other visualizations to support the research findings, making the paper more engaging and easier to understand.

5.2.3 Cons of ChatGPT

- **Lack of Personalization:** Generates generic responses that may not align perfectly with specific project requirements or personal learning styles.

- **Limited Contextual Understanding:** ChatGPT, while adept at generating responses based on a vast dataset, sometimes struggles with understanding the full context or nuances of a user's query. This limitation can lead to responses that, while technically accurate, might not fully address specific or nuanced project requirements. For instance, in a Senior Design project focusing on a highly specialized area of engineering, ChatGPT might offer general advice that doesn't fully grasp the project's unique challenges or specifications.

- **Inability to Conduct Real-Time Research:** Unlike traditional research methods or dynamic online search tools, ChatGPT cannot access or retrieve real-time information from the internet. This means it cannot incorporate the very latest studies, news, or innovations into its responses, which can be a significant drawback for projects that rely on cutting-edge technology or the most current data.

- **Potential for Plagiarism:** When generating text based on common knowledge and its training data, ChatGPT might inadvertently produce content that closely resembles existing sources. Students may unknowingly use such content in their projects, raising concerns about plagiarism and the authenticity of their work.

5.2.4 Cons of Google Gemini

- **Requires Specific Knowledge for Effective Use:** To leverage Google Gemini to its fullest potential, users need to have a good understanding of how to frame their search queries effectively. This learning curve can be a barrier for those less familiar with advanced search techniques, potentially leading to inefficient research practices and frustration.

- **Filter Bubble and Echo Chamber Effects:** Google Gemini, like other search engines, personalizes search results based on the user's previous searches, clicked links, and other online behaviors. This personalization can inadvertently lead to a filter bubble, where a user is only exposed to information and viewpoints that align with their existing beliefs or knowledge. In the context of a Senior Design project, this could limit exposure to a wider range of ideas, innovations, and critical perspectives.

- **Privacy Concerns:** Utilizing Google Gemini for research entails sharing search queries and potentially sensitive project information with Google's servers. For projects that involve proprietary information or are subject to strict privacy requirements, this could pose a risk. The concern over data privacy and the potential for intellectual property exposure must be considered when integrating Google Gemini into the research phase of a project.

5.3 Impact on Senior Design Learning Experience

1. **Enhanced Research Capability:** Both ChatGPT and Google Gemini significantly benefit the Senior Design learning experience by streamlining the research process. ChatGPT can quickly provide background information on a topic, while Google Gemini excels in finding current research articles. For instance, when tasked with integrating a novel technology into our project, Google Gemini provided the latest studies, whereas ChatGPT offered foundational knowledge.

2. **Improved Problem-Solving Skills:** ChatGPT aids in developing problem-solving skills by suggesting multiple approaches to a given challenge. For example, when encountering a design issue, ChatGPT proposed various solutions based on similar past projects, fostering a creative problem-solving mindset.

3. **Risk of Misinformation:** A notable drawback is the risk of relying on incorrect information from ChatGPT, which could lead to flawed project decisions.

4. **Over-reliance on Technology:** There's a risk of becoming too dependent on these tools, potentially hindering the development of independent research and critical thinking skills. For instance, over-reliance on Google Gemini for research may reduce engagement with primary sources, critical for a thorough understanding of the subject matter.

In conclusion, ChatGPT and Google Gemini offer substantial benefits to the Senior Design learning experience, particularly in enhancing research efficiency and fostering innovative thinking. However, awareness of their limitations and

potential drawbacks is crucial to mitigate risks associated with misinformation and over-reliance on AI tools. By judiciously leveraging these platforms in conjunction with traditional learning methods, students can significantly enrich their educational journey in Senior Design (OpenAI, 2024).

6 Design

6.1 Software Design

The software design for a Raman spectrometer involved developing a system that could control the instrument, acquire spectral data, process and analyze the data, and potentially interface with external devices or software for advanced analysis or data sharing. The software design is robust, flexible, and user-friendly to ensure efficient operation and accurate results and can be broken down by architecture, components, integration, and development.

Software Architecture Overview:

1. User Interface (UI)
    - The RAID spectrometer features a HAMTYSAN 8-inch Raspberry Pi Display touch screen interface where users interact to select the drink being tested and control various settings.
    - UI design includes touch response for starting, stopping measurements, and viewing results.

2. Control System
    - The Raspberry Pi 3 Model B+ microcontroller is the central operating system for the spectrometer.
    - The microcontroller interfaces with peripherals like the laser driver, spectrometer, photodiode, and HAMTYSAN 8-inch Raspberry Pi Display.

3. Data Acquisition and Processing
    - The software controls the spectrometer components for data acquisition.
    - Signal processing algorithms are employed to extract Raman spectra through the photodiode and compare them with reference spectra.
    - Algorithms analyze spectral data to detect the presence of specific substances.

Software Components in Detail:

1. User Interface (UI) Software
    - Developed using a graphical framework to ensure a responsive and intuitive touch interface.

- Allows users to initiate measurements, select beverage types, view results, and configure settings.

2. Control Software
   - Manages hardware components such as the laser diode, spectrometer, optical components, and photodiode.
   - Controls the laser diode driver to emit the 532nm laser light.
   - Orchestrates the movement of optical components like motors, mirrors, lenses, and filters based on measurement requirements.

3. Data Acquisition and Processing Software
   - Interfaces with the spectrometer's Czerny-Turner configuration.
   - Controls the rotation of the grating and the photodiode.
   - Processes raw spectral data to identify Raman shifts.
   - Compares acquired spectra against pre-loaded spectra of target substances (e.g., GABA) for identification.
   - Implements algorithms for real-time analysis and decision-making (e.g., presence/absence of target substances).

4. Result Display and Reporting
   - Shows analysis results on the LCD HAMTYSAN 8-inch Raspberry Pi Display in a user-friendly format.
   - Displays results of substance detection (positive/negative) and any relevant quantitative data.
   - Option to review historical data or export results for further analysis if required.
   - Shows detection status, estimated GABA concentration, and runtime
   - Features retest button responsible for restarting analysis of beverage sample
   - Including exit and logout buttons to exit RAID system software

Software Integration:

1. Hardware-Software Integration
   - Ensures smooth communication between software and hardware components.
   - Uses standardized protocols (e.g., SPI, I2C) to interface with sensors, actuators, and the spectrometer.

2. Real-time Performance
   - Optimizes software routines for real-time performance to enable rapid analysis and response.
   - Implements buffering and data streaming techniques for continuous data acquisition.

Deployment and User Interaction:

1. Field Deployment and Testing
    - Software tested to ensure reliability and accuracy in real-world, public environments like bars and clubs.
    - Calibration routines are integrated to maintain accuracy over time.

2. User Interaction and Accessibility
    - Focuses on ease of use and reliability to empower non-experts (e.g., bartenders) to utilize the device effectively.
    - Provides clear and actionable results to users through the touch-responsive LCD HAMTYSAN 8-inch Raspberry Pi Display.

Software Development Tools:

1. Programming Languages and Tools
    - Python for Raspberry Pi 3 Model B+ microcontroller programming
    - Python or similar for higher-level data processing and analysis.
    - Graphical user interface (GUI) framework including TKinter library for touch screen development.

2. Simulation and Testing Tools
    - Simulation tools (e.g., MATLAB/Simulink) for algorithm development and validation.
    - Testing frameworks for software verification and validation.

In conclusion, the software design of a Raman spectrometer is a process that involves integrating several crucial components to achieve accurate and real-time analysis of beverage samples for the presence of specific substances. By incorporating these considerations into the software design, a successful Raman spectrometer application capable of processing and analyzing high quality spectral data for beverage analysis can be developed.

6.2 Electrical Design

The electrical design of a Raman spectrometer is essential for its functionality and performance. This design involves several critical components that must be integrated carefully to ensure optimal power consumption and efficient operation. Central to the spectrometer's electrical system is the Raspberry Pi 3 Model B+, which acts as the central control unit. The Raspberry Pi coordinates the operation of the other components and processes the spectroscopic data. It is connected to an LCD HAMTYSAN 8-inch Raspberry Pi Display, providing a user-friendly interface for displaying spectroscopic data and control parameters.

To facilitate Raman spectroscopy, the spectrometer includes a laser driver and a laser. The laser driver controls the laser's operation, which is used to excite the sample and induce Raman scattering. The laser driver is connected to the Raspberry Pi for control and synchronization.

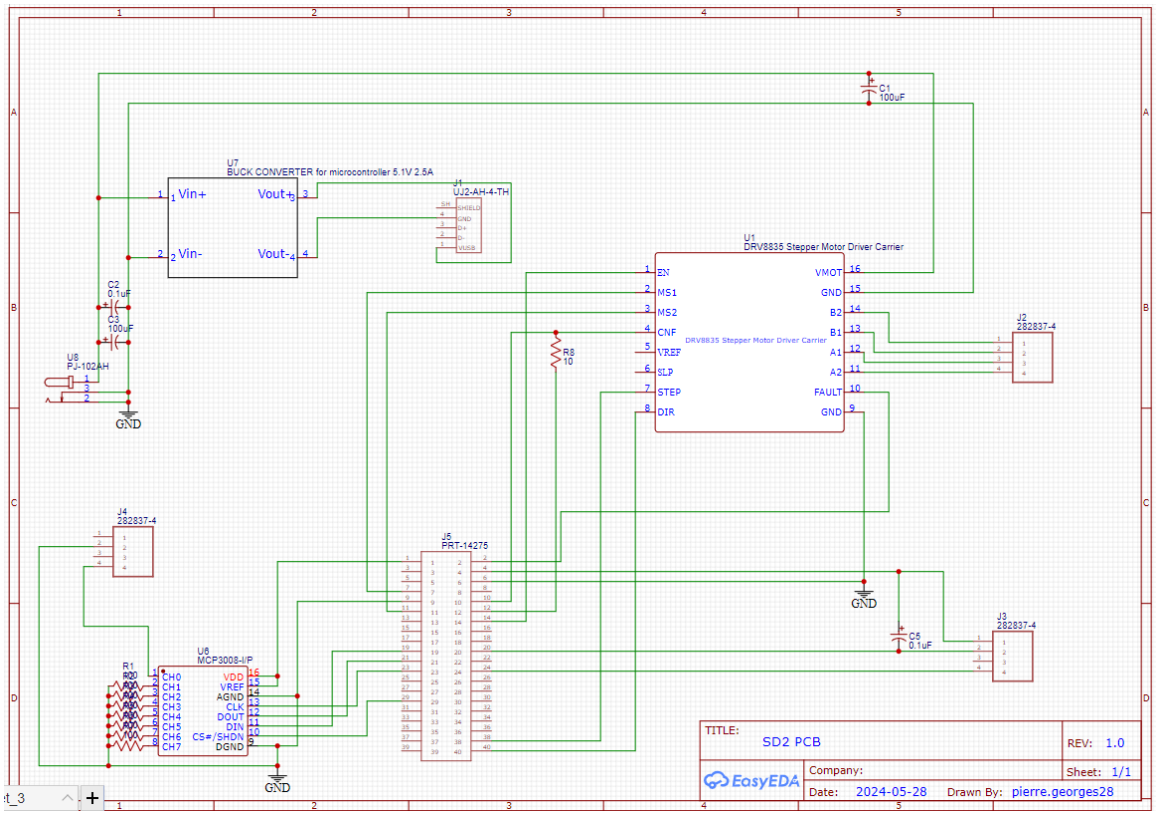
In addition to the laser, the spectrometer features a rotating stage consisting of a NEMA 14 stepper motor and a DVR8825 stepper motor driver. These components allow for precise control of the sample's position and orientation, enabling accurate spectroscopic measurements.

Power management is a critical consideration in the design of the spectrometer. The Raspberry Pi, LCD display, laser driver, and stepper motor driver all require a stable power supply to function correctly. The design process included determining the voltage and current demands of each component and selecting an A/C power wall adapter that could provide the necessary power. This adapter supplies 5 volts and enough current to meet the demands of all components simultaneously.

Interconnections between the components were carefully planned to ensure smooth communication and operation. The Raspberry Pi communicates with the LCD display via an HDMI interface for displaying spectroscopic data and control parameters. The laser driver is connected to the Raspberry Pi through GPIO pins, allowing the Raspberry Pi to control the laser's operation. Similarly, the stepper motor driver is connected to the Raspberry Pi for controlling the rotation of the stage.

In addition to the components mentioned, the design also includes a custom PCB to streamline the electrical connections and ensure reliability. The PCB design was carefully considered to accommodate the various components and their interconnections. It will be designed to be compact yet robust, allowing for easy integration into the spectrometer's overall design.

In conclusion, the electrical design of a Raman spectrometer is a complex process that requires careful consideration of various factors, including power consumption, interconnections, and PCB design. By ensuring proper integration and coordination of these elements, we will be able to deliver a reliable Raman spectrometer that users can count on for accurate beverage analysis.



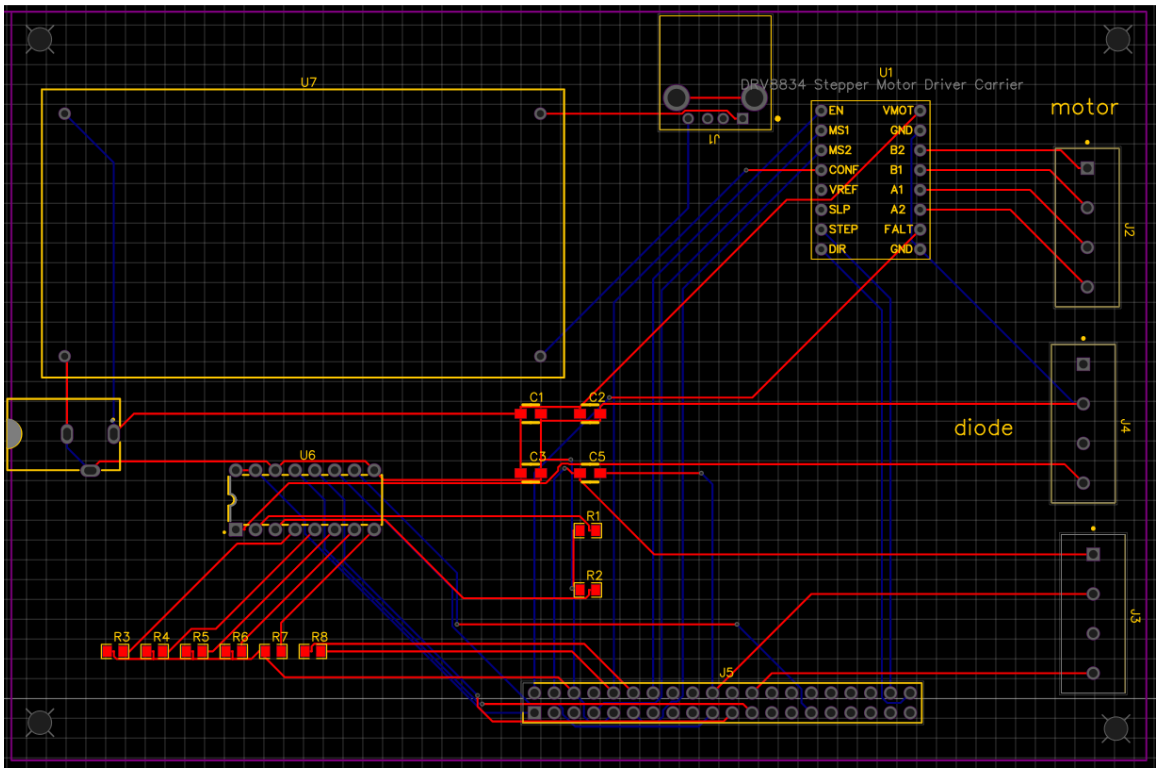


Figure 6.2.1 Electrical Design

7 System Testing and Evaluation

System testing and assessment are critical components of the RAID project's development and refinement, providing significant insights into the spectrometer's performance and capabilities.

During the last demonstration of the optical illumination system, both encouraging progress and unanticipated obstacles emerged. While the apparatus did successfully record a signal, it was not at the expected wavelength. Instead of the expected center wavelength of GABA's Raman spectral peak of roughly 580nm, a peak at 804nm was discovered. Despite this variance, a minor movement from 804 to 805nm was observed, showing possibilities for future optimization and calibration.

Dr. LikamWa given helpful advice based on these findings to improve the spectrometer system's performance. One significant proposal was to increase the quantity of laser light directed at the sample. Using a continuous wave to pulse the sample with maximal laser power could result in a greater Raman signal than pulsing the beam with a square wave using a function generator. Given that we were operating only at 100 mW during the demonstration, we are able to operate at 500 mW which would significantly increase the signal received from our spectrometer. Furthermore, optimizing the optical components by choosing lenses with a higher numerical aperture (NA) and a shorter focal length may assist conserve as much signal and light as possible as it travels through the system. These proposals emphasize the significance of fine-tuning system parameters for peak performance and sensitivity.

Furthermore, the inclusion of an avalanche photodiode in the spectrometer system was suggested as a potential approach to improve signal detection. Avalanche photodiodes have higher sensitivity and lower noise characteristics than standard photodiodes, making them ideal for detecting weak optical signals like Raman scattering. By incorporating this advanced detector technology into the system, the RAID project might potentially improve its signal-to-noise ratio and detection sensitivity, improving overall performance and dependability.

In addition, the feasibility of using a linear array as an alternate detector was investigated as a backup plan. If issues develop with photodiode alignment or performance, switching to a linear array detector may be a potential alternative. This solution would eliminate the requirement for a stepper motor rotation stage, simplifying the system architecture and possibly boosting dependability and ease of use. The RAID project aims to ensure robust performance and adaptability in a wide range of operating circumstances and scenarios by considering multiple signal detection and system optimization possibilities.

7.1 Spectrometer Design Optimization

System testing and assessment are essential components of the spectrometer optimization process, which aims to fine-tune the system parameters for maximum performance and sensitivity. To do this, we obtained two distinct lenses, each with its own set of features, and tested their effectiveness in gathering dispersed light from the grating and focusing it onto the avalanche photodiode. The major goal is to increase signal collection while keeping the wavelengths identifiable. We prefer the 25 mm focal length lens since it allows us to keep the device compact and portable. However, if this lens proves to be ineffective, we can address the issue with a 50 mm lens, albeit at a loss of signal power and system size.

Additionally, we have implemented two slits within the spectrometer setup to further refine our testing and evaluation process. The first slit, positioned in front of the spectrometer, serves to capture the dispersed light or Raman signal. This slit also plays a crucial role in determining the spectral resolution of the spectrometer by controlling the width of the light beam reaching the detector. By adjusting the slit width, we can strike a balance between spectral resolution and the amount of light reaching the detector, thereby optimizing the performance of the spectrometer for our specific application. The second slit, located in front of the avalanche photodiode, enables us to selectively choose the wavelengths for investigation, necessitating collaboration between the photonics engineering student overseeing the spectrometer and the computer engineering student responsible for spectrum analysis and LCD display integration.

A critical aspect of system testing involves identifying the most prominent peaks in the Raman spectra of GABA and aligning the grating on the rotation stage to the appropriate angle to capture the desired wavelengths. This meticulous adjustment increases the likelihood of detecting a GABA Raman spectral signal, thereby enhancing the quality of detection and quantification of GABA concentrations.

However, the optimization process also requires continuous realignment of the system to ensure that laser light is preserved as it passes through the spectrometer. This iterative approach necessitates a large time and labor investment, as thorough changes and frequent testing are required to reach and maintain peak system performance. By methodically testing and developing each component of the spectrometer system, we want to maximize its sensitivity, precision, and reliability for GABA concentration detection and analysis in a variety of applications.

In order to optimize the performance of our RAID spectrometer system, we are using powerful simulation tools such as Zemax to undertake thorough studies of photodiode active area needs. Recognizing that different wavelengths focus on somewhat different spots, we want to make sure that the photodiode we choose

has the right size, sensitivity, and Noise Equivalent Power (NEP) to successfully capture dispersed light across the spectrum. Using Zemax's sophisticated capabilities, we can map out the optical properties and performance metrics of several photodiode alternatives, allowing us to make informed decisions during the selection process.

We intend to use Zemax simulations to mimic the behavior of several photodiode active regions under varied situations and wavelengths, allowing us to analyze their sensitivity and signal-to-noise performance across the spectrum of interest. This method allows us to discover the best photodiode design for balancing sensitivity and spectral resolution, resulting in accurate and reliable Raman signal detection. By methodically examining the simulation results, we can determine the optimal photodiode active area size for maximum signal detection while minimizing noise, hence improving the overall performance and sensitivity of our spectrometer system.

7.2 GABA Concentration Optimization

According to the United States Pharmacopeia (USP), the human dose quantity for GABA, a neurotransmitter supplement commonly utilized for its alleged calming properties, is normally approximately 750mg to produce significant results. Given this dose threshold, it is critical that the RAID system detect GABA concentrations at or above this level reliably. Detecting quantities less than 750mg may be ineffective because they do not generate visible effects in persons, particularly bar patrons who may have been unwittingly exposed to spiked beverages. Thus, the spectrometer's sensitivity must be properly adjusted to identify clinically relevant GABA concentrations and potential tampering.

To accomplish this basic goal, significant testing is required to evaluate the spectrometer's ability to identify GABA in a variety of liquid samples effectively. While water can be used as a baseline for testing, the RAID system should also be assessed with other typical liquids present in bars, such as alcohol and juices, to account for potential changes in matrix effects and sample compositions. This extensive testing procedure ensures the system's durability and applicability in a variety of environments and scenarios where contaminated drinks may occur.

When assessing GABA concentrations, spectrometer performance must be optimized to increase signal strength and sensitivity. Testing raw GABA samples allows for the refining of measurement methodologies and parameters to reliably determine the strongest signal from solid GABA samples. By adjusting the system's settings and methods for solid samples, the RAID system can ensure the highest signal intensity when analyzing liquid samples, improving its capacity to identify GABA concentrations precisely and reliably.

Therefore, verifying the RAID system's ability to detect GABA concentrations at or over the human dosage threshold of 750mg is critical to its efficiency in

detecting spiked drinks in bars. Through rigorous testing and optimization techniques across multiple liquid samples, the RAID system can verify its reliability and accuracy in detecting GABA, increasing its utility as a tool for ensuring drink safety and reducing potential harm to bar guests.

7.3 Rotating stage testing

Testing the NEMA 14 stepper motor for the motorized stage in our Raman spectrometer was crucial to ensure its functionality and compatibility with the overall system. We begin by verifying the electrical connections of the stepper motor, ensuring correct connections to the stepper motor driver and power supply. Using a multimeter to check the continuity of the wiring and confirm that there are no short circuits.

Functional testing was the next step. Using the stepper motor control library, we tested the motor functionality. The NEMA 14 motor responded to commands to move a certain number of steps in one direction and then in the opposite direction. Observation yielded smooth and consistent movements.

The motor was then attached to the motorized stage that holds the grating lens and applied a load that simulates the weight of the lens. The same commands were sent to the motor to move the stage back and forth, ensuring it could move the load smoothly without skipping steps or losing position. This load testing was essential to validate the motor's performance under operating conditions.

The motor's temperature was monitored during operation using a thermal sensor. Stepper motors can become hot during operation, so it is essential to ensure that they do not overheat. The motor was run for an extended period to test its temperature and ensure it stayed within safe limits. An endurance test was also conducted to ensure the motor could operate continuously for an extended period without issues. The motor ran for several hours, monitoring its performance and temperature throughout the test.

After these testing procedures, we felt that the NEMA 14 stepper motor for the motorized stage in our RAID Raman spectrometer met the required specifications and performed reliably under various conditions.

7.4 System Testing Results

Our RAID team data tested a sample containing 1000 mg of GABA. During the first round of analysis, the information displayed on the GUI confirmed there was GABA detected in the sample with an estimated concentration of 1000 mg which was correct. However, during the next iteration a false negative was generated with a differing graph. We retested the same 1000 mg sample 10 times and found

that our system has a detection status accuracy rate of 80% with an estimation accuracy rate of 40%.

Changes in detection status of the same sample could be attributed to slight variations in sensor readings of the MCP3008 ADC and signal processing each time the sample is retested. Photodiode sensitivity, noise, environmental factors, and electronic fluctuations can cause these inconsistencies even with the same sample.

We encountered several issues with photodiode sensitivity affecting our results including noise interference from the usage of a USB port on the PCB. Using a camera in place of a photodiode would have offered better accuracy in our results and reduced the chance of noise or interference as the camera is a quicker and simpler solution but due the constraints of this class, we had to ensure enough work for two computer engineers by using a photodiode and motor.

Based on research to ensure more consistent results, we could have:

1. Increase the number of samples averaged to reduce noise. - However, we are already at 800 samples and an increase in samples could affect runtime.
2. Implement data smoothing or filtering techniques. - The Savitsky Golay smoothing method in place and implemented in our program but we could further increase the value.
3. Ensure stable environmental conditions during measurements.

Going forward if we had an opportunity to do this project again, we would use a camera to communicate the results with the GUI instead or spend more time on photodiode calibration and narrowing down if other system components are interfering with our system producing more accurate results. Although we faced some issues with estimations and photodiode sensitivity, we were overall able to produce a system with the intention of determining if GABA is present in a drink using a photodiode and motor set up with a certain level of accuracy.

8 Administrative Content

Administrative content is a vital aspect of project management, providing key information essential for effective oversight and decision-making. This section includes details such as the project budget, the Bill of Materials, and Senior

Design II milestones. While these elements may not directly influence the technical aspects of engineering design, they are paramount for ensuring our project's success and adherence to its objectives.

8.1 Budget

Budget information within the administrative content outlines the financial resources allocated for the project. This includes initial budget estimates and cost breakdowns for materials and services. The budget sets a target that ideally should not be exceeded. In our case, we budgeted approximately $700. Each member was responsible for procuring their respective components.

Table 8.1.1 Project Budget

Item	Quantity	Budget
Gamma-aminobutyric acid (GABA)	1	$10
532nm laser diode	1	$60
Dichroic Mirror	1	$75
Longpass filter	1	$185
15mm lens Ø12.7mm	2	$80
Lens	2	$80
Pinhole	1	$15
Photodiode (VTB4051H)	1	$20
LCD	1	$20
PCB + components	1	$50
TCD1304DG	1	$37
Rotating Stage	1	$41
Microcontroller	1	$15
Total Cost		$675

8.2 Bill of Materials (B.O.M.)

The bill of materials (BOM) for the RAID Raman Spectrometer is a comprehensive list of all the parts and components purchased for the development of the device. This list includes all the necessary materials required for both the design and testing phases of the project, ensuring that the device meets its performance and functionality requirements.

Table 8.2.1 Bill of Materials

Item	Supplier	Part Number	Quantity	Cost
Gamma-aminobutyric acid (GABA)	Bulk Supplements	N/A	1	$18.96
532nm laser diode	MKS Instruments	N/A	1	Free
Dichroic Mirror	MKS Instruments	DCM13	1	$342
Longpass filter	MKS Instruments	20CGA-550	1	$102
25mm EFL Lens	MKS Instruments	KPX076AR.14	2	$42.00
38mm EFL Lens	MKS Instruments	KPX046AR.14	1	$42.00
250mm EFL Lens	MKS Instruments	KPX109AR.14	1	$43.00
50mm EFL Lens	MKS Instruments	KPX082AR.14	1	$43.00
Slit	MKS Instruments	SV-0.5	1	$347.00
Homemade Slit	RAID Team	N/A	1	Free
Photodiode	Excelitas	VTB4051H	1	Free
CCD	Digikey	TCD1304DG (8Z, K)	1	$37.00
Pinions Gears	Hobbyfire	54T 32P	1	$13.95

Stepper motor driver	Bigtree	TCM2209	1	$11.88
Stepper motor	Stepperonline	14HS13-0804S	1	$15.91
Microcontroller	Amazon: Raspberry Pi Foundation	2842229	1	$46.00
LCD Display Screen	Amazon: HAMTYSAN Store	KST-8INCH01	1	$65.49
ADC converter	Amazon: Bridgold	MCP3008	1	$6.99
Raspberry Pi case	Amazon: SB Components Store	780746862598	1	$5.99
MicroSD Card	Amazon: SanDisk	SDSQUNC-128G-GN6MA	1	$14.39
Optomechanical Components (misc.)	MKS Instruments/ RAID Team	N/A	4	$300
Total Cost				$1497.56

8.3 Milestones

The creation of the following tables is to establish solid deadlines for our group throughout the upcoming two semesters. This initiative ensures collaborative efforts, fostering cohesion among team members in understanding task timelines. The RAID team has built a schedule to streamline our workflow which can be seen below:

Table 8.3.1 Senior Design 1 Documentation Milestones

Task	Start Date	Anticipated End Date	Duration
Project Conceptualization	Fall	Spring	1 month
Formation of Group	01/08/2024	01/11/2024	3 days

Project Idea Finalization	01/05/2024	01/12/2024	1 week
Assign Roles of Project/ Research Tasks Associated	01/15/2024	02/02/2024	2 weeks
Divide and Conquer Report Writing (10-Page Milestone)	01/15/2024	02/02/2024	2.5 weeks
Discuss Progress in Group Meeting (30-Page Milestone)	02/05/2024	03/21/2024	2.5 weeks
60-Page Milestone	02/05/2024	03/29/2024	3.5 weeks
Discuss Progress in Group Meeting (90-Page Milestone)	04/05/2024	04/14/2024	1.5 weeks
Final Document (120-Page Milestone)	04/01/2022	04/23/2024	2.5 week

Table 8.3.2 Senior Design 1 Project Design Milestones

Task	Start Date	Anticipated End Date	Duration
Components Selection	01/24/2024	02/24/2024	1 month
Discuss Selections with Advisors	02/25/2024	03/02/2024	1 week
Components Finalization	03/03/2024	03/29/2024	3.5 weeks
Purchasing Components	03/30/2024	04/30/2024	1 month

Table 8.3.3 Senior Design 2 Fabrication Milestones

Task	Start Date	Anticipated End Date	Duration
Motorized Rotation Stage	05/15/2024	05/22/2024	1 week

Raman Capturing Testing	05/15/2024	05/29/2024	2 weeks
Spectrometer Testing	05/15/2024	06/07/2024	3 weeks
System Integration	05/29/2024	06/26/2024	3.5 weeks
Mock Demo (to find and fix issues that arise)	07/03/2024	07/17/2024	2 weeks
Upload Final Documentation	07/17/2024	07/23/2024	1 week
Final Presentation	07/19/2024	07/19/2024	1 day

8.4 Work Distributions

The work distribution table below outlines the tasks and responsibilities for each team member involved in the development of the Raman Analyzer for Illicit Drugs. This information is crucial for ensuring accountability and efficient project management. Each team member is assigned specific tasks and is responsible for completing them in a timely manner. In case a team member is unable or unwilling to complete a task, there is a designated backup person who will take over the responsibility.

Task Allocation lies at the heart of this approach. By assigning specific tasks to each team member, the table establishes clarity regarding who is responsible for what. This eliminates confusion and ensures that team members know exactly what is expected of them, thereby minimizing the risk of duplicated efforts or tasks slipping through the cracks.

Responsibility and Accountability are cornerstones of this method. Each team member is accountable for their designated tasks. This accountability fosters a sense of ownership and commitment to delivering quality work within the allocated timeframe. Knowing that they are individually responsible for their part motivates team members to perform at their best and meet project milestones.

Timely Completion is emphasized throughout the table. Each team member understands the importance of completing tasks within the specified timeframe. This ensures that the project progresses smoothly and stays on schedule. Team members are motivated to work efficiently to avoid delays, keeping the project momentum intact.

Contingency Planning is integrated into the table. The inclusion of backup persons for each task serves as a safety net in case of unforeseen circumstances. This proactive approach minimizes the impact of potential setbacks and maintains continuity in project execution, ensuring that tasks can be seamlessly reassigned without disrupting progress.

Holistic Project Coverage is ensured by the table's meticulous outlining of tasks and responsibilities. From research and development to testing and documentation, every phase of the project has dedicated team members overseeing it. This comprehensive coverage minimizes the risk of overlooking crucial elements and ensures a well-rounded approach to project execution.

Efficient Resource Utilization is a key benefit of this approach. By assigning tasks based on individual strengths, skills, and expertise, the table optimizes resource utilization. Each team member contributes where they can add the most value, maximizing productivity and enhancing the overall quality of deliverables.

Facilitating Communication is another advantage provided by the clarity of the work distribution table. Effective communication within the team is facilitated, as team members can easily coordinate, collaborate, and provide updates on their progress. This ensures transparency and alignment towards common project goals.

This work distribution ensures that each aspect of the project is covered by a responsible team member, with a backup plan in place to ensure tasks are completed even if someone is unable to do so. This approach helps maintain project momentum and ensures that all project requirements are met within the specified timeframe.

Table 8.4.1 Work Distribution

Task	**Champion** **P - Primary** **S - Secondary**	**Task**
Light source	P: Nicole Parker	Selection and implementation of light source
Illumination path	P: Nicole Parker S: Michael Soto	Optical path from light source to water
Light collection	P: Michael Soto S: Nicole Parker	Ensure alignment of Raman signal towards photodiode

Spectrometer Grating	P: Michael Soto	Disperse light into distinct wavelengths
Data processing	P: Asha Waters	Process spectral data from microcontroller
Data output	P: Asha Waters	Show results on touchscreen display
Electrical design - powering	P: Pierre Georges	PCB design to power all components
Rotating Stage	P: Pierre Georges	Design grating bill rotating stage
RAID Device	ALL	R&D, design and implementation of Raman Spectrometer

8.5 Declaration of Originality

We hereby declare that we have not copied more than 7 pages from the Large Language Model (LLM). We have utilized LLM for drafting, outlining, comparing, summarizing, and proofreading purposes.

Appendix

This section contains all the referenced materials utilized in the design and creation of this document. As illustrated below, all the essential information required to replicate this document and project is available.

Appendix A Works Cited

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