Raman Analyzer for Illicit Drugs (RAID)

Group 2 Nicole Parker Michael Soto Asha Waters

Jean Georges

RAID

Team Composition:



Nicole Parker Photonic Engineer



Asha Waters Computer Engineer



Michael Soto Photonic Engineer



Jean Georges Computer Engineer





GOALS

- 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.



OBJECTIVES

- 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.



Specifications Total bootup time 2 minutes Spectral resolution < 1nm Total runtime ~20 secs Spectral range 550nm – 790nm 750 mg Lowest concentration measured ± 0.01 mm to ± 0.1 mm Motor accuracy Computer interface Touch screen Touchscreen responsivity 5 ms

SPECIFICATIONS AND REQUIREMENTS

DESIGN APPROACH AND IMPLEMENTATION

This Raman Spectrometer is composed of two parts: (1) the excitation and collection stage and (2) the Czerny Turner spectrometer

RAID was designed to be used in bars, clubs, and any other venue where roofies are of concern.

SYSTEM DESIGN

System Design

Spectrometer

Raman Illumination and collection

Sample Chamber and UI





Optical Design







HARDWARE COMPONENTS

Grating Selection





Model #: 33066FL01-560R Ruled Reflective Diffraction Grating

Transmissive Diffraction	Reflective Diffraction
Gratings	Gratings
Transmits most light.	Reflect all incident light; modulate
Absorption causes possible light	undesired components. Excellent
loss; impacts signal strength.	at maintaining polarization control.
Requires precise alignment in optical systems to ensure optimal performance and accuracy.	Effectively redirect incoming light in the direction of the detector to make the most of the available light and improve signal detection.
Typically, "in-line," requiring longer optical paths. Ideal for minimizing optical distortion and maximizing spectrum resolution in imaging systems, fluorescence spectroscopy, and some optical microscopy.	Common, flexible, compact, and effective optical setups. Used in Raman spectroscopy and some optical imaging systems for focusing dispersed light onto a detector or focal point.

Photodiode Selection





DET 210 — High Speed Si Photo Detector

	Specifications
Detector	Silicon PIN
Spectral Response	200 - 1100nm
Peak Wavelength	730nm+/-50nm
Rise/Fall Time	1 NS
NEP	5 E-14 W/sqrt(Hz)
Active Area	1mm
Output	BNC, DC Coupled biased with 12V battery
Cost	\$181.68



Excitation Source

Common Raman Pump Wavelengths

Pump Wavelength (nm)	Laser Type	Application/Advantages	Disadvantages	
532	Diode-Pumped Solid-State Laser (DPSS)	High sensitivity, good for visible range applications	Fluorescence interference can be significant	
633	Helium-Neon (HeNe) Laser	Lower fluorescence interference compared to 532 nm	Lower Raman scattering efficiency compared to 532 nm	
785	Diode Laser	Reduced fluorescence, good for biological samples	Lower spatial resolution, lower scattering efficiency	
830	Diode Laser	Further reduced fluorescence, good for dark samples	Even lower scattering efficiency, more expensive	
1064	Nd Laser	Minimal fluorescence, good for highly fluorescent samples	Significantly lower Raman scattering efficiency, expensive	

Final Decision: 532 nm @ 500 mW



Longpass Filter Options

Feature	MKS Newport 20CGA-550	Thorlabs FELH0550	Edmund Optics #47-505
Size	50.8x <u>50.8mm</u>	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



MKS Newport 20CGA-500



Beam Splitting Mechanism

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	>ø <u>11.43mm</u>	8.8mm	



MKS Newport DCM13



Lens Choices

	Lens	Purpose
1	KPX046AR.14 EFL 38.1	Focus pump onto sample and collimate Raman signal
2	KPX043AR.14 EFL 25.4	Focus beam into fiber
3	KPX082AR.14 EFL 50.2	Collimate signal from fiber to spectrometer
4	EFL 50	Focus into photodiode

Beam measurement – 1.2mm

DataRay 8.06081.ive	e image 49 of 64 Exp@18.	288mm Filter	-0.2% Wi-	670.0vm, Parel	-11.00:11.00, in	nage - 2048 by 20	46, Fest Came	na #1 (CTE/HyperCal on)	
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Features	STM32 Nucleo- F401RpyET6	Raspberry Pi 3 Model B+	Arduino Uno	
Processor	32-bit ARM Cortex-M4 core, up to 84 MHz	1.4 GHz 64-bit quad core ARM Cortex-A53	16 MHz	
RAM	512 KB	1 GB	2 KB SRAM	
Drive Space	512 KB Flash	32 GB Flash, microSD card	32 KB Flash	
Input Voltage	3.3 - 12 V	5.1 V DC	7 - 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 Options

Key Features of Our Selection:

- 1.4 GHz processor
- Larger computing power
- Increased memory & storage
- Community support available for troubleshooting



Display Options

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	OLED 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



Key Features of Our Selection:

- Touchscreen capability
- Larger display size
- Quick responsiveness
- Multitouch functionality
- Compatible with Raspberry Pi 3 Model B+ microcontroller selection

Bridgold MCP3008 ADC

- Resolution: 10 bit
- Channels: 8 analog input channels
- SPI Interface
- Sampling Rate: maximum rate of 200 kilosamples per second (ksps) based on operating conditions
- Voltage Range: 2.7 V to 5.5 V
- Low power consumption



Allegro Microsystems ACS712 Current Sensor

- Current Sensing Range: ±30 A
- Output Voltage Sensitivity: 66 to 185 mV/A
- Supply Voltage: 4.5V to 5.5V
- Operating Temperature Range: -40° C to 85° C
- Output Type: analog
- Bandwidth: close to 80 kHz



Motorized Stage

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

Feature	A4988	TMC2209	DRV8825	
Manufacturer	Allegro MicroSystems	BigtreeTech	Texas Instruments	alle -
Max Current per Phase	2A	2.5A	2.5A	
Operating Voltage	8V - 35V	8.2V - 45V	8.2V - 45V	Son As
Micro-stepping	Full, Half, 1/4, 1/8, 1/16 steps	Full, Half, 1/4, 1/8, 1/16, 1/32, 1/64, 1/256 steps	Full, Half, 1/4, 1/8, 1/16, 1/32 steps	and the second
Overcurrent Protection	Yes	Yes	Yes	1000
Overtemperature Protection	Yes	Yes	Yes	1 Aug
Suitable Applications	General purpose projects	Projects requiring higher resolution and smoother motion	Projects requiring higher resolution and smoother motion	
Compatible with Arduino	Yes	Yes	Yes	
Compatible with Raspberry Pi	Yes	Yes	Yes	



Motorized Stage

Desired step angle = 0.005° Selected gears: Pinion: 13T 48P Driven gear: 90T 48P

Overall Gear Ratio = 6.923Effective step Angle = 1.8° Effective step angle with 1/64 Microstepping = $1.8^{\circ}/64 \approx 0.028125^{\circ}$ Final step angle $\approx 0.00406^{\circ}$





Schematics





Schematics





Sheet_3









Budget

Part	Unit	Unit Price	Total Amount
20CGA-550 Longpass Filter	1	\$102.00	\$0.00
33066FL01-280R Ruled Diffraction Grating	1	\$176.00	\$0.00
DCM13 Beam Combiner	1	\$342.00	\$0.00
DGF-12 Diffraction Grating Mount	1	\$44.00	\$0.00
KPX046AR.14 EFL 38.1 Lens	1	\$42.00	\$0.00
KPX043AR.14 EFL 25.4 Lens	1	\$42.00	\$0.00
KPX082AR.14 EFL 50.2 lens	1	\$43.00	\$0.00
EFL 50 Lens	1	-	\$0.00
M1Q Mirror Mount	1	\$46.00	\$0.00
M-PPF50 Filter Mount	1	\$112.00	\$0.00
SV-0.5 Adjustable Slit	1	\$347.00	\$0.00
532nm 500mW Laser + Driver	1	-	\$0.00
MMF NA 0.27 Optical Fiber	1	-	\$0.00
Fiber Mount	2	-	\$0.00
Lens Mount	2	-	\$0.00
Mirrors	2	-	\$0.00
Mirror Mount	3	-	\$0.00
Rotation Stage	1	-	\$0.00



Budget

Part	Unit	Unit Price	Total Amount
Post + Post Holder	10	-	\$0.00
Optical Clamping Fork	8	-	\$0.00
Screws	-	-	\$0.00
Photodiode	1	\$181.68	\$0.00
Cuvette 4pc	1	\$36.99	\$36.99
Gamma Aminobutyric Acid Powder (GABA supplement)		\$18.96	\$18.96
Raspberry Pi Container	1	\$5.99	\$5.99
Raspberry Pi 3 Model B+ Board	2	\$46.00	\$92.00
HAMTYSAN 8 Inch Touch Screen	1	\$65.49	\$65.49
SanDisk MicroSD Card	1	\$14.39	\$14.39
MCP3008 ADC Converter	1	\$6.99	\$6.99
ACS712 Current Sensor Detector	1	\$3.25	\$3.25
NEMA14 Motor	1	\$15.91	\$15.91
Stepper Motor Driver	1	\$11.88	\$11.88
Gears	1	\$13.95	\$13.95
PCB Components	1	\$30.97	\$30.97
Power Supply Adapter	1	\$11.99	\$11.99

Budget



	Unit Price	Total Amount
Total Price	\$1,760.44	\$328.76

Thanks to MKS Newport for sponsoring the optical components!

SOFTWARE COMPONENTS

Software Overview



OBJECTIVE: Develop a graphical user interface to run an algorithm that process the data captured and determines the presence of GABA, notifying the user whether beverage is safe or spiked.



Operating System:

Raspberry Pi OS also known as Raspbian



Integrated Developed Environment (IDE):

Visual Studio Code

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Programming Language:

Python



Raspberry Pi OS Key Features

- Optimized for Raspberry Pi Hardware
 - Ensuring maximum compatibility and performance
- Pre-installed software & development tools
 - Including Python which saves time during initial setup
- Extensive documentation
 - Making it easier to develop & troubleshoot applications
- Security updates
 - OS has regular security updates ensuring the application environment is secure
- Efficient
 - Consumes minimal resources such as memory and processing power



RELATED STANDARDS

Standards



Standard	Reason
ISO 9001:2015 – Quality Management	It helps organizations of all sizes and sectors to improve their performance, meet customer expectations and demonstrate their commitment to quality.
IEC 60825-1:2014 – Safety of Laser Products	To introduce a system of classification of lasers and laser products emitting radiation in the wavelength range 180 nm to 1 mm according to their degree of optical radiation hazard in order to aid hazard evaluation and to aid the determination of user control measures

DESIGN CONSTRAINTS

- Ethical Considerations:
 - Ensuring accurate detection to avoid false positives/negatives which could have serious implicatior

• Health and Safety:

- Due to its controlled substance nature, illicit drugs were not readily available for testing.
- PPE is required when assembling or troubleshooting due to laser.
- User Training:
 - Providing comprehensive training for users to ensure safe and effective operation.
 - Clear instructions and user-friendly design to minimize user error.
- Energy Efficiency:
 - Due to time constraints and limited know how our prototype is not the most energy efficient.
 - More R&D would yield more efficient methods to accomplish said goal.
- Manufacturability:
 - Limited knowledge of mounting optics outside of the breadboard.
- **Economical and Time:**
 - Because these spectrometers are complex and precise, we are limited to what we can include in our design's



SUCCESSES AND DIFFICULTIES

Successes and Difficulties



PCB

- Success: Learning how to solder
- Difficulty: Noise and electromagnetic interference

Motorized Stage

- Success: Integrating the NEMA14 with the stepper driver
- O Difficulty: Getting down to the 0.005° required to rotate the grating lens

Spectrometer

- Success: Aligning the optical components to the system
- O Difficulty: Integrating the stepper motor rotation stage into the system

GABA Analysis

- Success: Installing necessary software needed to run program via microcontroller
- O Difficulty: Converting analog signal from photodiode to digital signal for microcontroller

CHALLENGES FACED COMPLETING RAID PROJECT



Challenges Faced During Completion

The Creation of the Housing

- Due to our lack of Mechanical Engineering experience with CAD, we struggled designing a housing.
- Given that we are building a spectrometer for Raman Spectroscopy, we need to be very precise when aligning our RAID systems. Aligning on our systems without the use of an optical breadboard (creating our own by hand) served as a MAJOR challenge. Given the time and cost constraints, we had to use wood rather than aluminum to recreate the optical breadboard.

• Photodiode Calibration:

• Struggled to determine the proper algorithm necessary to analyze the Raman signal we were receiving.

Rotation Stage Calibration:

- Determining a way to calibrate the motor, grating, and wavelength was difficult to find a solution for. We ended up using a Helium and Neon lamp which has peaks that are between 500 600 nm which is close to where our GABA peaks lie (around 580 nm).
- Building a step motor with such a small resolution (0.005-degree steps)

If we had more time...



• Find a lighter housing alternative to enable better portability.

Calibrate the photodiode properly.

Try testing with different substances.

Questions?

