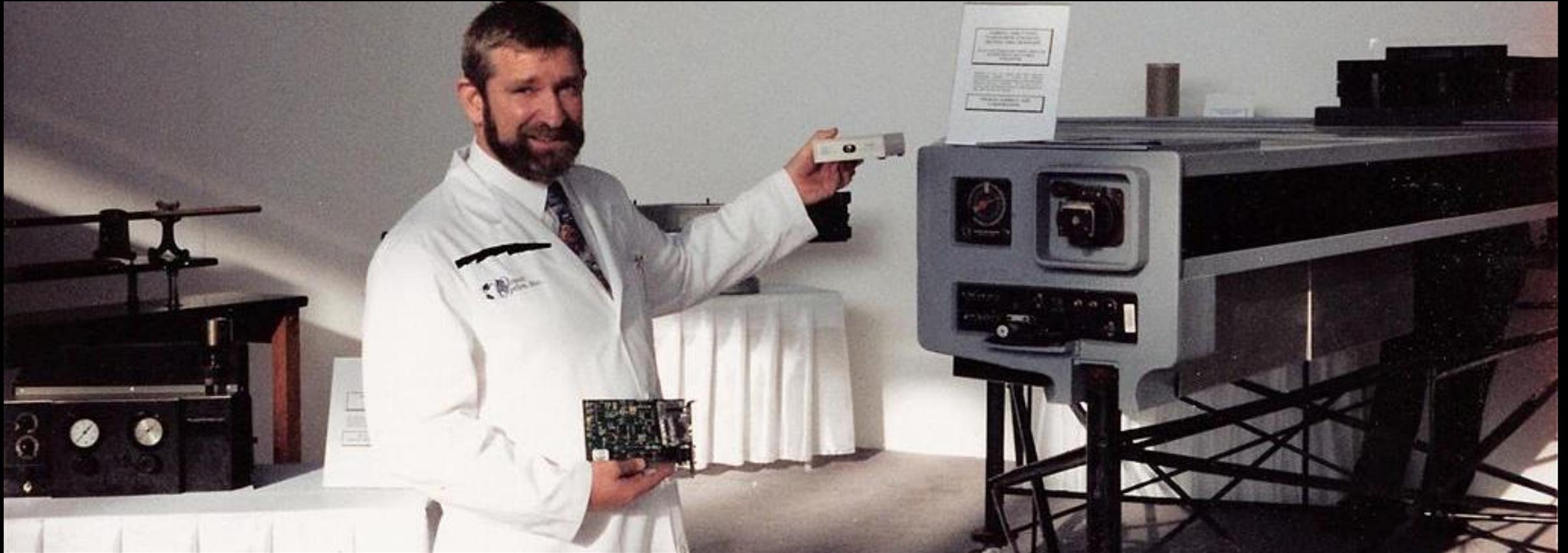


Introduction

- Welcome and Thank You from Dr. Steve Buckley and Derek Guenther
- Topics To Be Covered:
 - Recent Advances in Spectroscopy Hardware and Software
 - Power of Machine Learning in Spectroscopic Solutions
 - Advances and Applications of Imaging Systems

Ocean: Partnering with research and industry



Spectrometers, Light sources, Multispectral cameras, Machine learning, Raman, LIBS, Device development and manufacturing ...

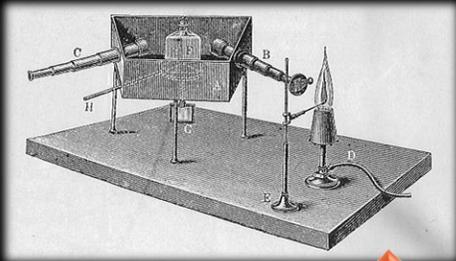


Ocean Optics → Ocean Insight

A short explanation...

Recent Advances in Spectral Systems

- On the cusp of 2020 looking back, spectroscopy has come a long way!



Wikimedia Commons



Libretext, 2019



Srismrita Basu, 2017



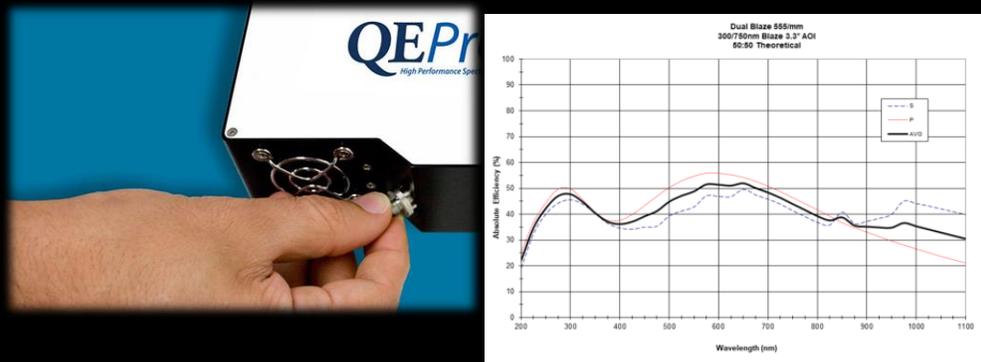
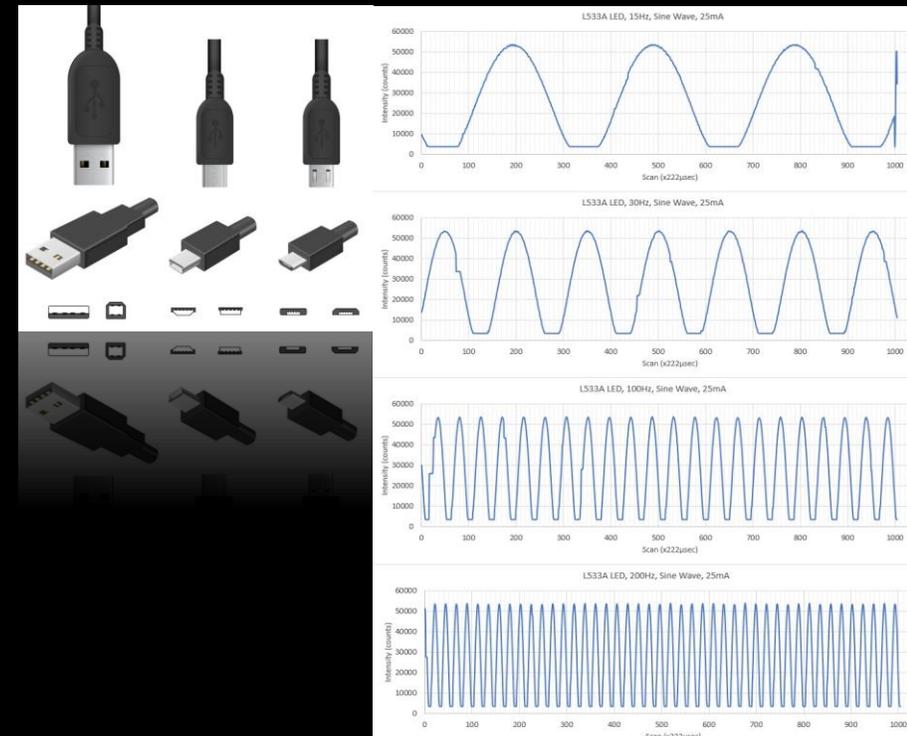
Anabolic Lab



- Systems are smaller and more intuitive
 - A benefit of many worlds (*disciplines*) colliding!

Recent Advances in Spectral Systems

- Which worlds have collided?
 - Spectroscopists, ME's/OME's, EE's, ChemE's, SE's, *Artists and Designers*
 - Designs become more clever with each discipline added
 - Communication teaches us tricks we would not have known otherwise
 - Some Examples:
 - Interchangeable Slits (**OME + Spectroscopist**)
 - Ports and Communication Updates (**SE + EE + IE**)
 - Extended Range Gratings (**OME**)
 - High-Speed Acquisitions (**SE + EE**)
 - Auto-Integration Time and others (**SE + EE**)



Spectrometer Bench Design Improvements

- Improved Mirror Designs

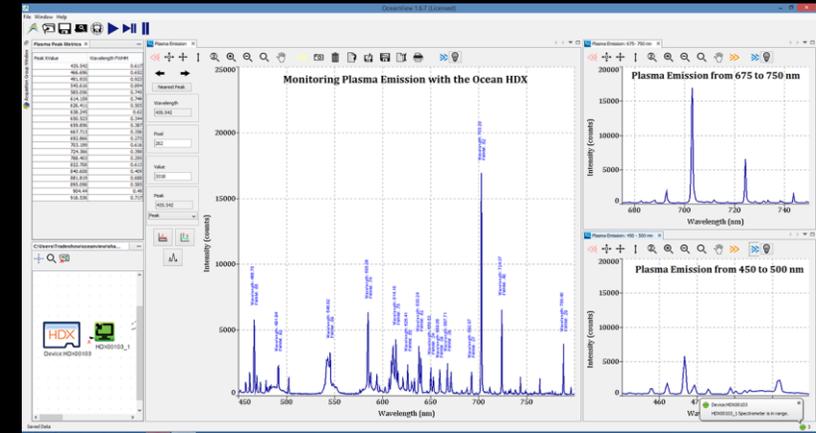
- Traditional mirrors can be improved: Geometry + Material
- Higher Resolution: Better separation of narrow emissions
- Peak Symmetry
- Throughput: Sensitivity for low level fluorescence / Raman

- Internal Structures

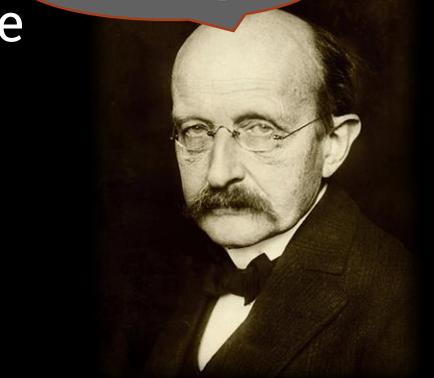
- *Where science and creative design come together! And with much benefit!*
- Lower Stray Light: Increased maximum absorbance / usable dynamic range

- Back-Thinned Detectors

- Greater UV Sensitivity

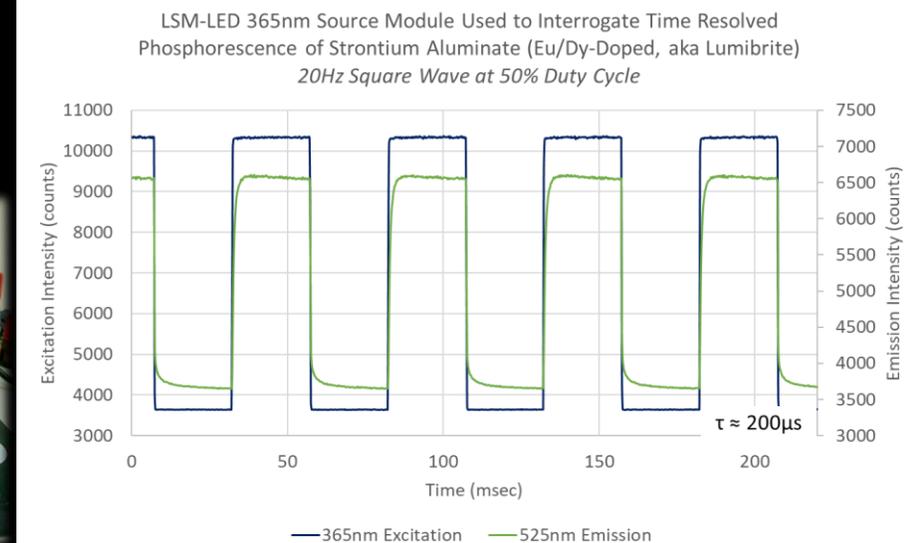
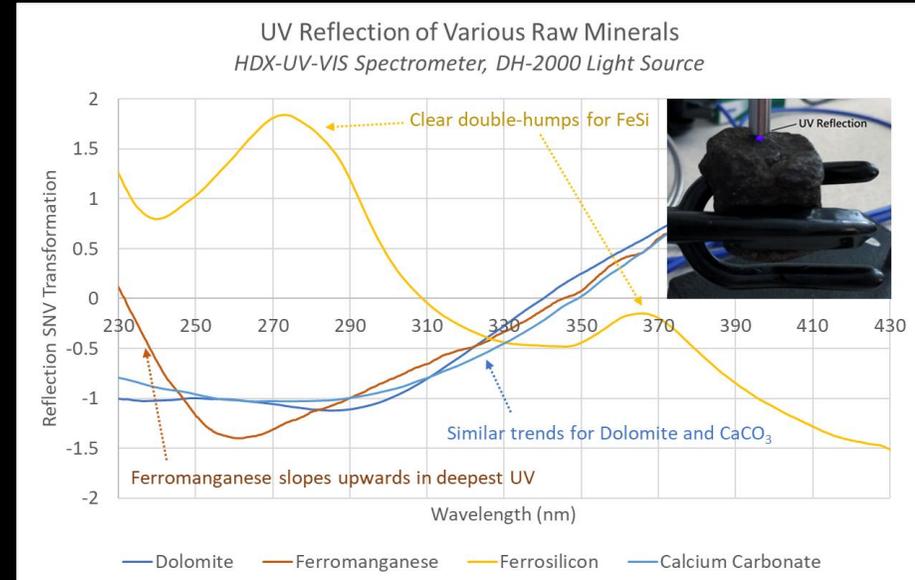


Baffling!



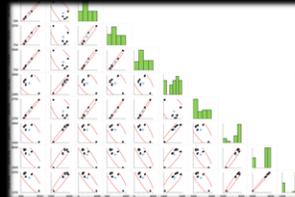
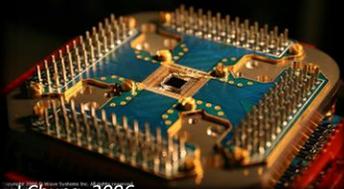
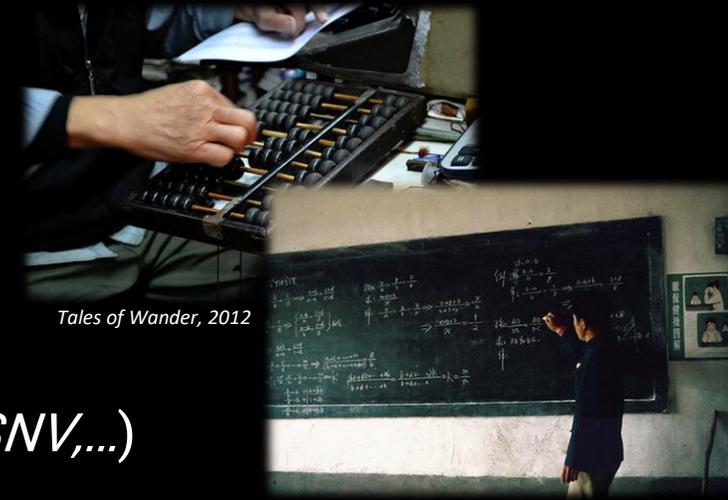
Spectrometer Bench Design Improvements

- Applications Made Possible By Improvements:
 - Trace-level detection of industrial fluorescent markers
 - Extended concentration ranges for highly absorbing samples
 - High-resolution Raman and LIBS measurements with small device footprint
 - UV/VIS/NIR broadband analysis in a single device
 - Sub-millisecond acquisitions for time-resolved broadband analysis of lighting, phosphorescence, and others



Advances in Spectroscopy Software

- Spectral Processing of the Past:
 - Manually dig through raw spectra
 - Arrange and process (Abs/Ref/Trans)
 - Visually identify activities
 - Pray these trends fit $mx+b$
 - Employ time-consuming techniques (*baselining, smoothing, SNV,...*)
 - Repeat analysis
- Modern Processing Power + Software Tools = *Turbo* Analytics



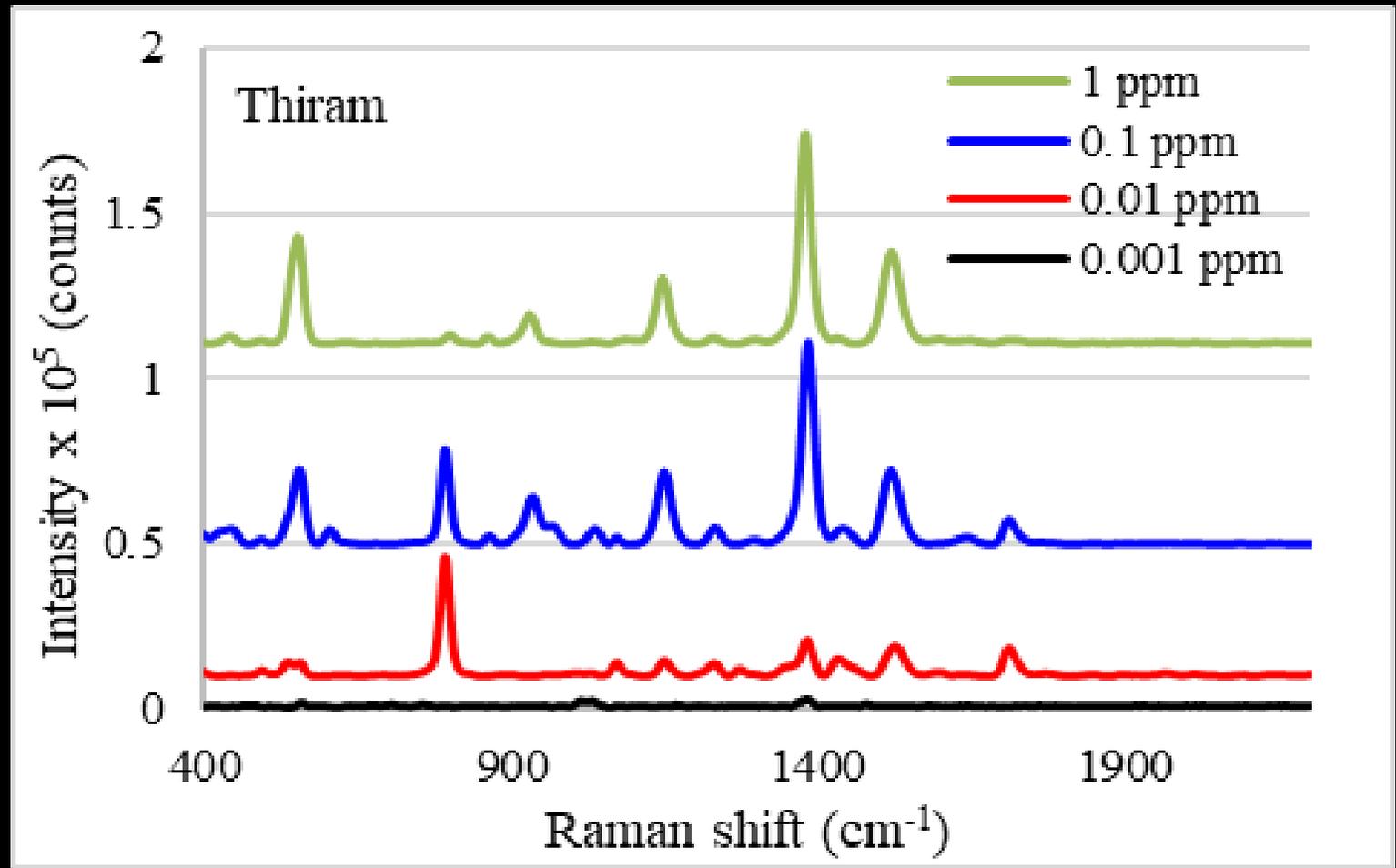
Multivariate

Advanced Regressions

- YouTube + Wikipedia + Time To Kill = Everyone is an 'Expert' Dilettante

Application: Raman for pesticide residue detection

- Surface-Enhanced Raman Spectroscopy (SERS)
- Known amount of sample mixed with known SERS volume for absolute concentration



Application: Trace Pesticide Detection Using SERS

- Detection of 21 pesticides using Surface Enhanced Raman Spectroscopy (SERS)
- Fungicides / Insecticides
 - Neonicotinoids / Organophosphates / Others
- Human Concerns: Parkinson's link
 - Environmental Concerns: Bee / Butterfly Decline
 - Secondary Human Concerns: *Crop Yields w/o Pollinators???*
- Gold Nanoparticles Engineered for Enhancement
 - Swab Fruit → Liquid-Phase Measurement
- Pure Pesticide LOD's: 0.001 – 10 ppm

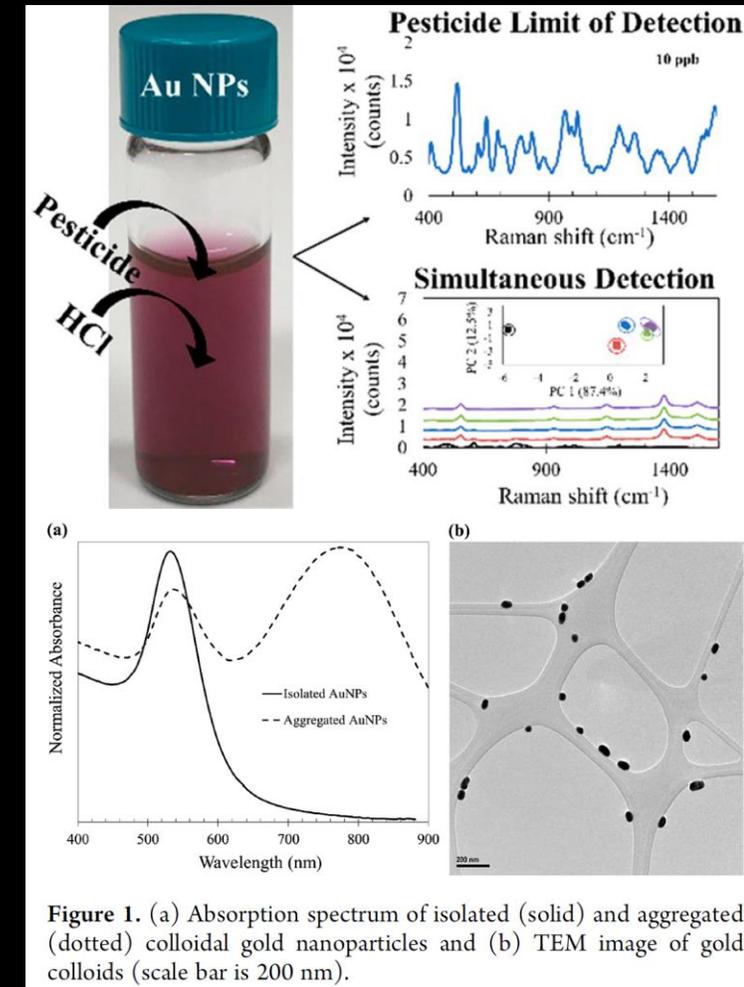
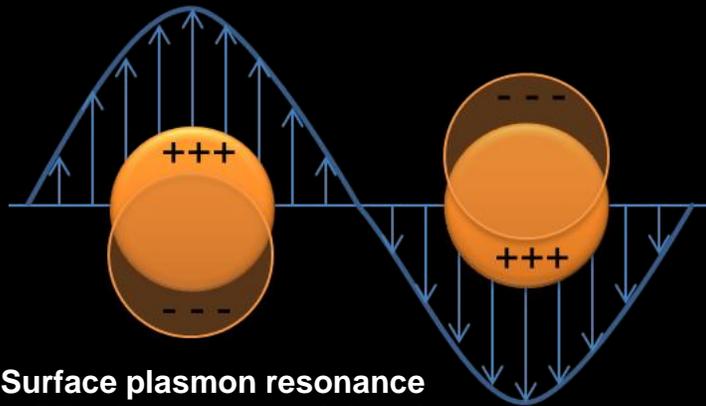


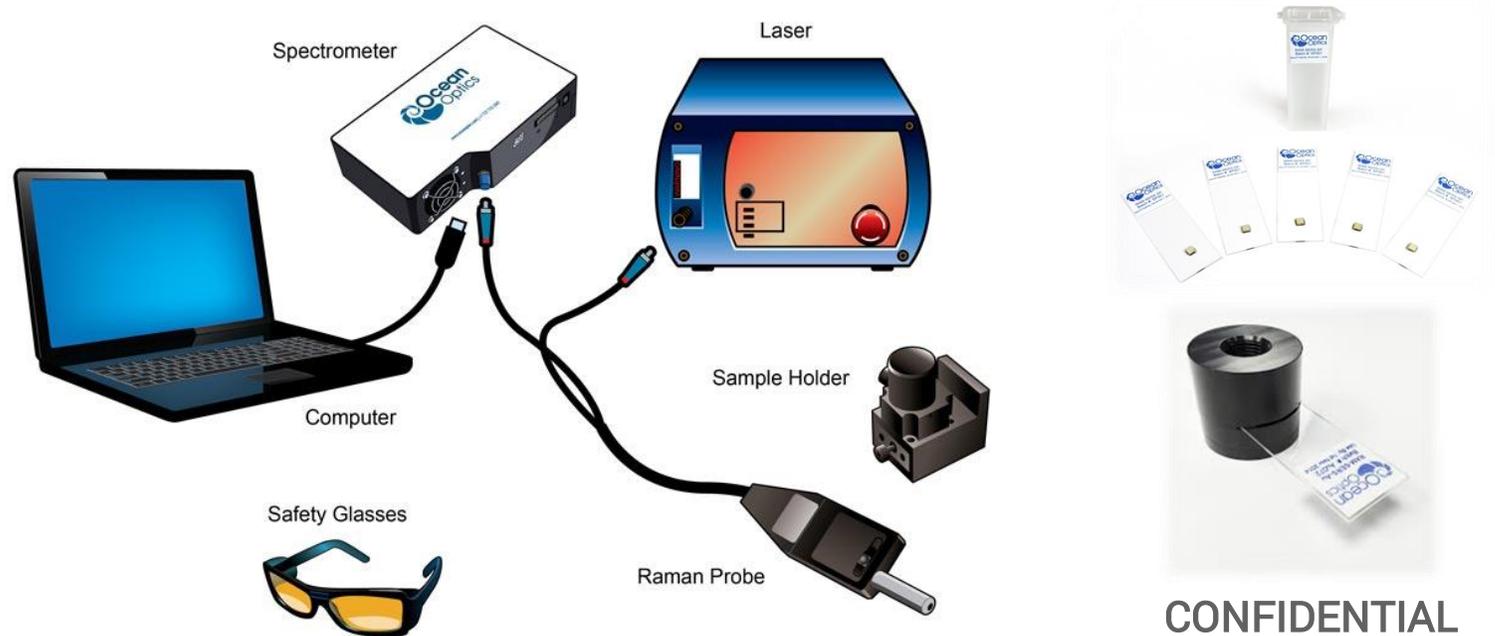
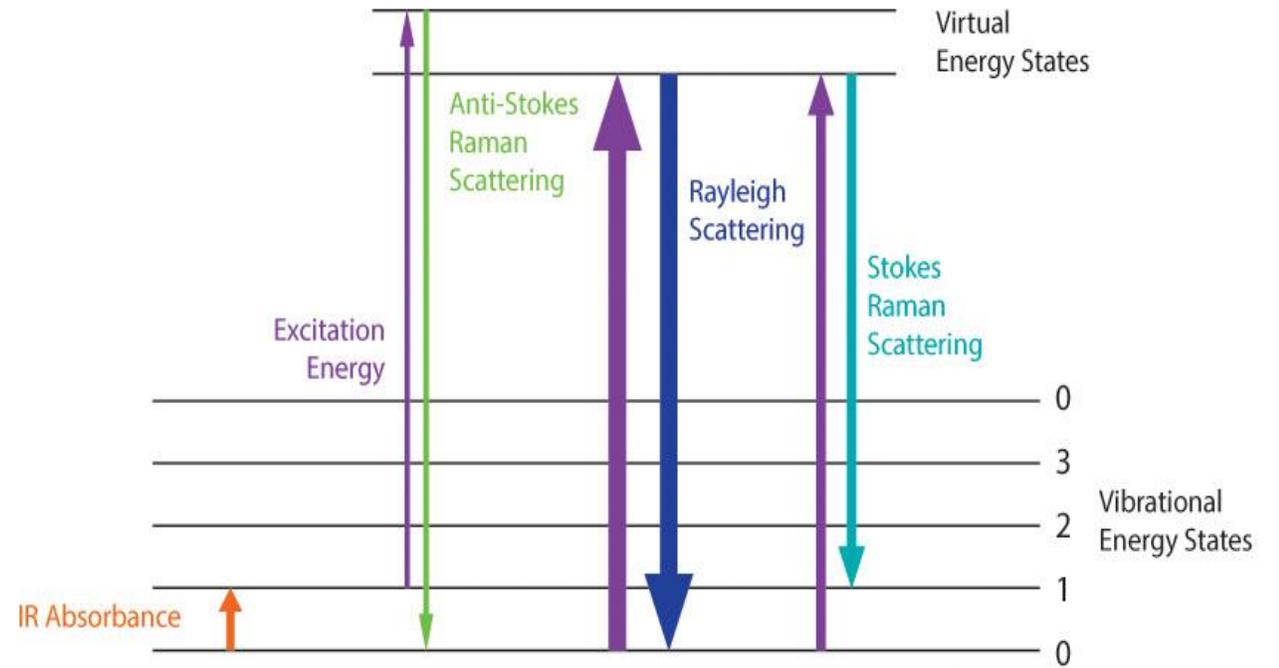
Figure 1. (a) Absorption spectrum of isolated (solid) and aggregated (dotted) colloidal gold nanoparticles and (b) TEM image of gold colloids (scale bar is 200 nm).

Application: Trace Pesticide Detection Using SERS

Theory Snapshot and Example Setup



Surface plasmon resonance (SPR) phenomena exhibited by metal nanoparticles



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Application: SERS Raman Detection Limits

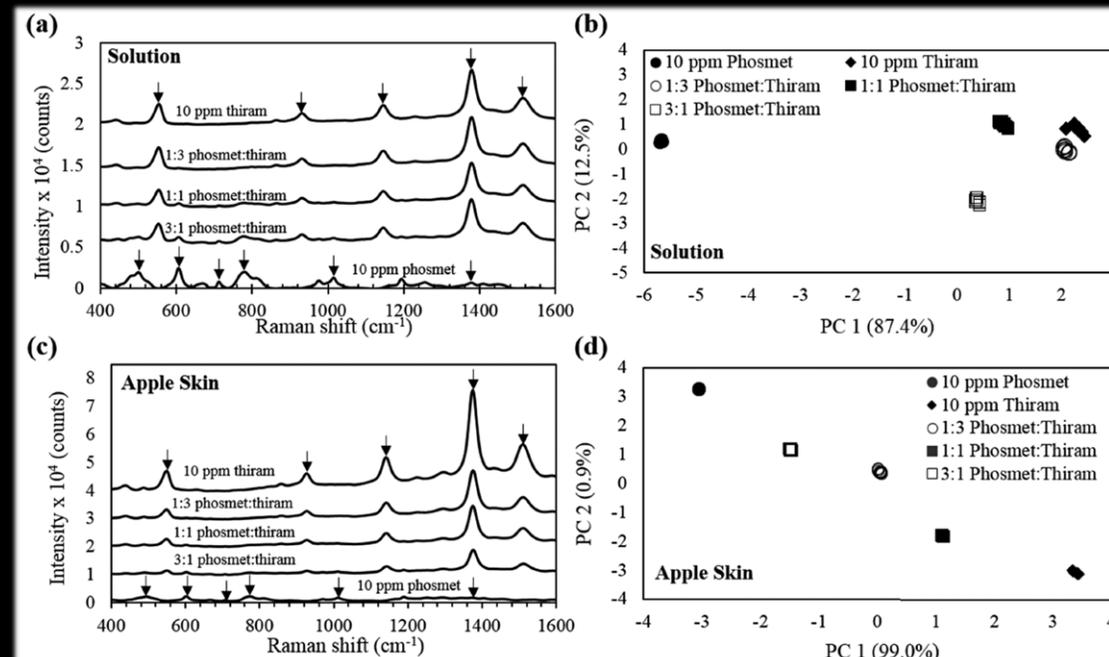
Pesticide	LOD (ppm)
Fungicides	
Diphenylamine	0.01
Fludioxonil	0.1
Thiabendazole	0.1
Thiram	0.001
Miscellaneous insecticides	
Carbofuran	0.01
Methomyl	0.1
Permethrin	0.001
Transfluthrin	1
Trichlorfon	0.001

Determination of the Limit of Detection of Multiple Pesticides Utilizing Gold Nanoparticles and Surface-Enhanced Raman Spectroscopy

A. M. Dowgiallo and D. A. Guenther
Journal of Agricultural and Food Chemistry Article ASAP
 DOI: 10.1021/acs.jafc.9b01544

Application: Trace Pesticide Discrimination Using SERS and Machine Learning

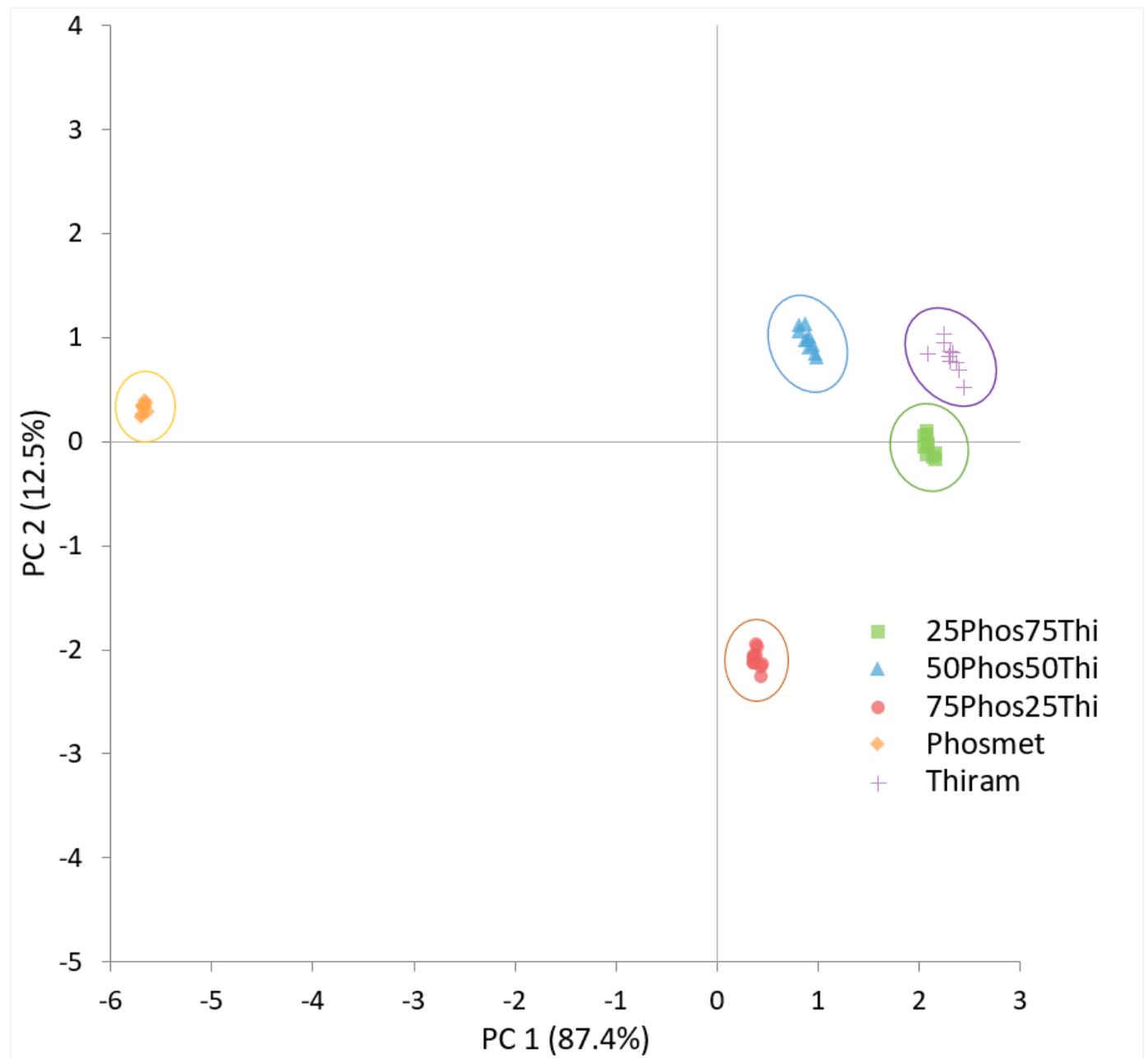
- Apple skins coated with:
 - 10ppm phosmet / 10ppm thiram
 - 1:3, 1:1, 3:1 ratios
- PCA to show statistical differentiation, even between mixtures



Application: Trace Pesticide Discrimination Using SERS and Principal Component Analysis

- So we see benefits from:
 - Hardware Improvements
 - Cross-Discipline Collaboration
 - Power of Numerical Software Tools

...but there's a step beyond



Machine Learning Meets The Mainstream

- First machine learning concept: Arthur Samuel (IBM) 1952
 - Computer learned winning checkers strategies
 - IBM kept momentum with Watson Jeopardy win
- A.I. Voice Recognition
 - Yesterday: Handled your car insurance calls (poorly)
 - Today: Your personal assistant (*Alexa, Siri, Cortana*)
- A.I. Image Recognition
 - Google's 'X Lab': Software browsed internet, identified things
 - MS currently making attempts with images imported to this PPT

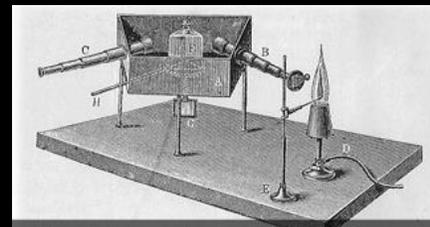


History-Computer, 2019



BigThink, 2011

- 1800's Spectrometer → '*Sewing Machine*'



Alt Text: A picture containing sewing machine,...

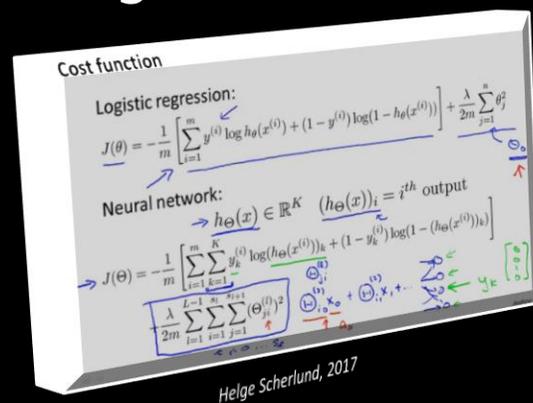
- 1900's Spectrometer → '*Microwave*'



Alt Text: A hand holding a microwave...

Machine Learning Meets Spectroscopy

- Pattern Matching Goes Beyond Photographs
- Numerical Methods Shared & Developed Across Disciplines
- Algorithm Packages Made Available via Purchase + Shareware



python



MATLAB & SIMULINK



Azure



- Methods Applied to Spectral Data Sets

Machine Learning Meets Spectroscopy

- Benefits Immediately Clear *...and then some*
- Computer can handle pre-processing:
 - Smoothing, baselining, statistical transformations
 - Identifies regions of activity vs. stability vs. noise
- Takes analysis one, or several, steps further

01

Identification/
Classification

Determine what the user is looking at for sorting purposes or alarm/warning

Spectra → *Decisions*

02

Concentration

Output numerical answer the end user is looking for

Spectra → *Answers*

03

Prediction

Anticipate some future value or condition based on recent or deeper historical trends

Spectra → *Foresight*

04

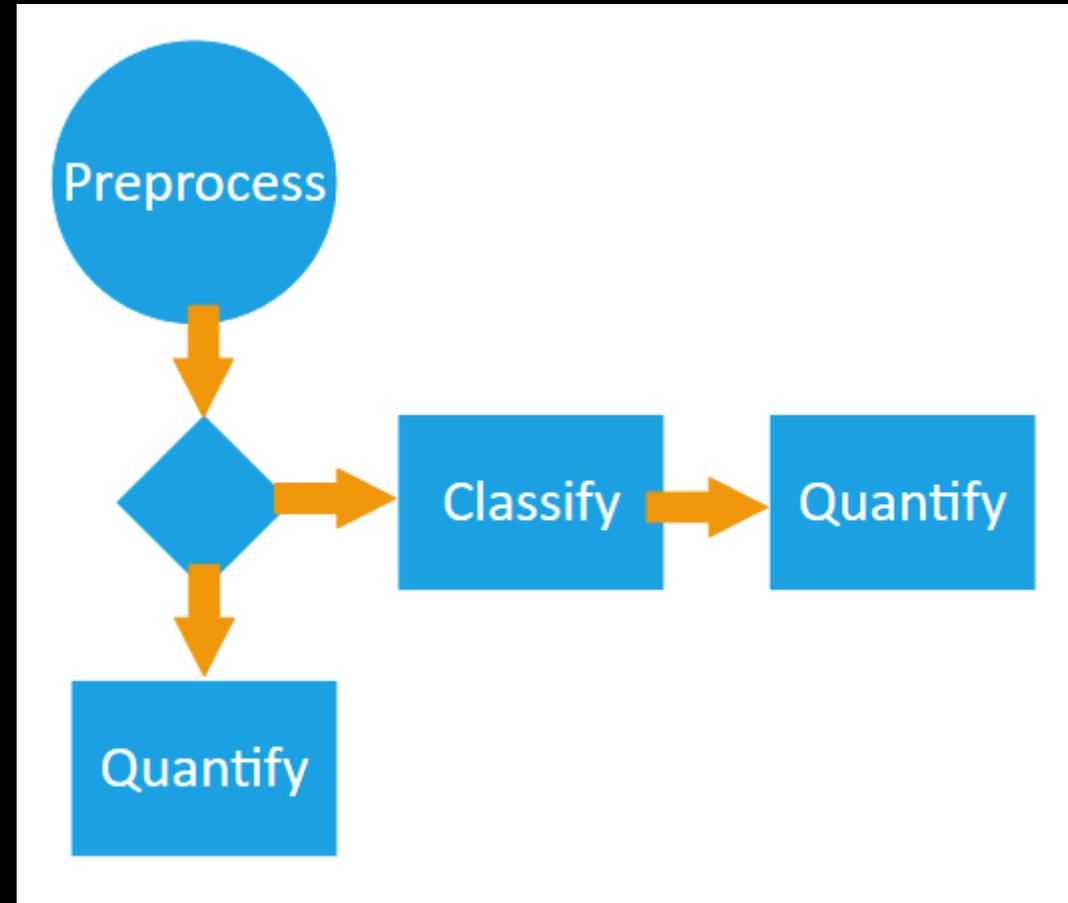
Calibration

Update process calibration data based on historical models

Spectra → *Assurance*

Basic answers from machine learning

- Classification of type
- Prediction of quantifiable value
- Combinations of classification and quantification



Toolset of “Chemometrics” has been greatly expanded by explosion of machine learning

- Term coined by Svante Wold in 1971
- Bruce Kowalski (University of Washington CPAC) and Wold founded International Chemometrics Society
- Original methods were multivariate regression and classification
 - Principal components analysis, regression
 - Partial least squares
 - Clustering

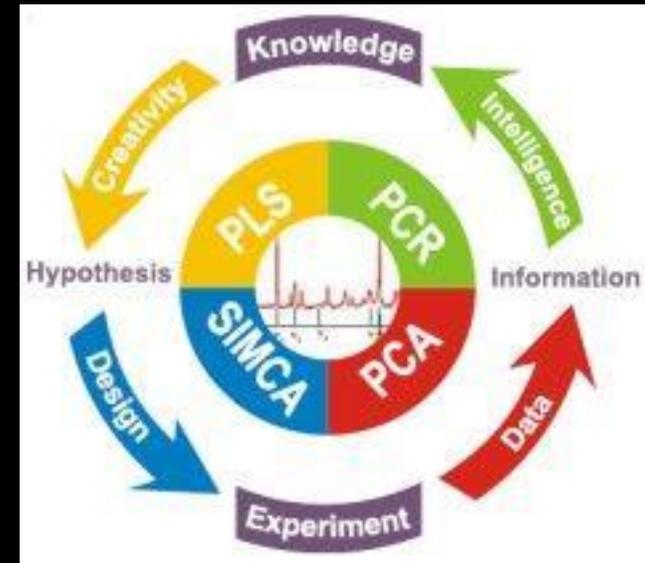
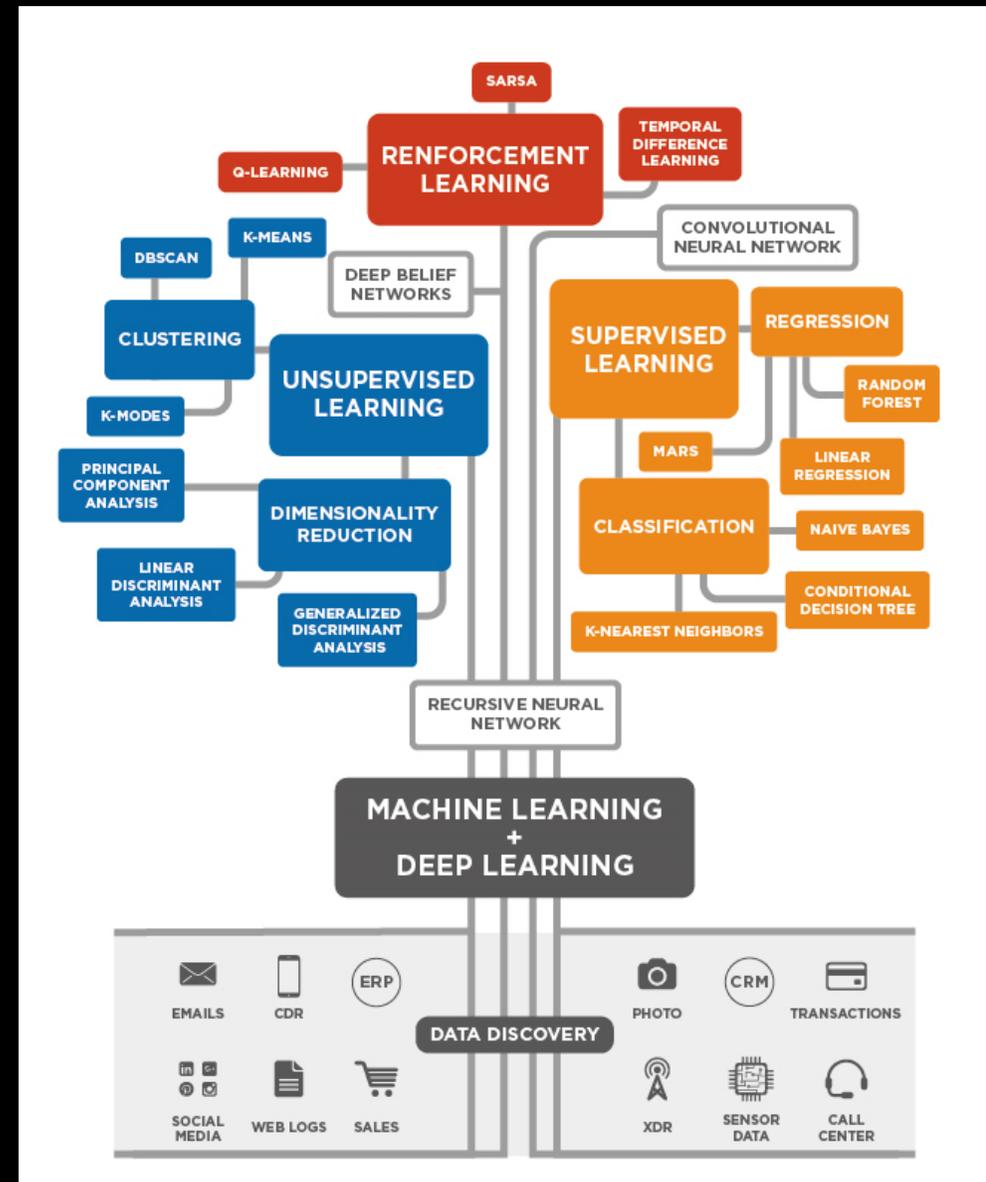


Image from www.camo.com

(Camo is a leading provider of chemometric software)

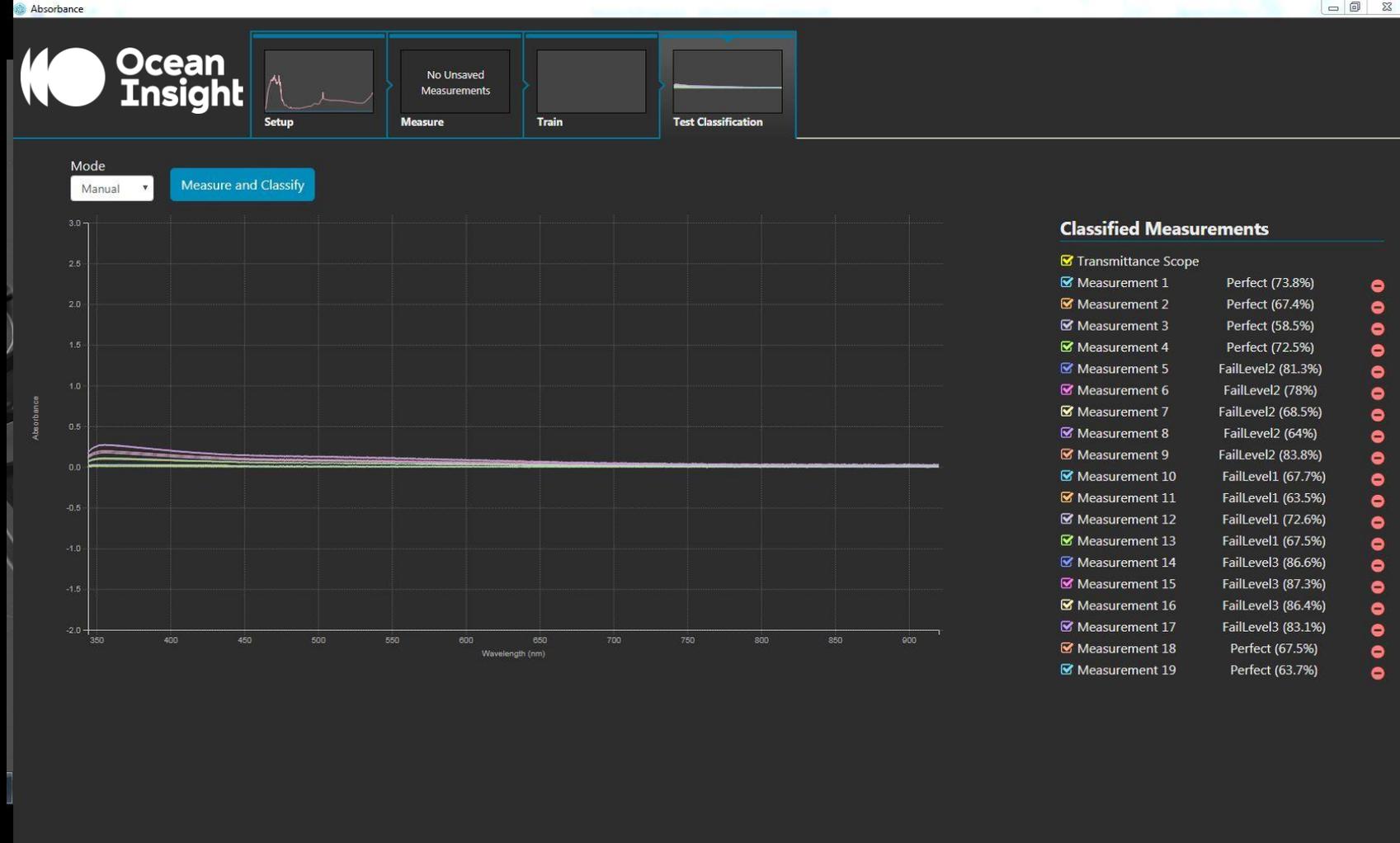
The Repertoire and Uses of Machine Learning have exploded

- Many data inputs
- A large number of supervised and unsupervised data analysis methods
- “Ocean Intelligence”



Applications in Spectral Machine Learning

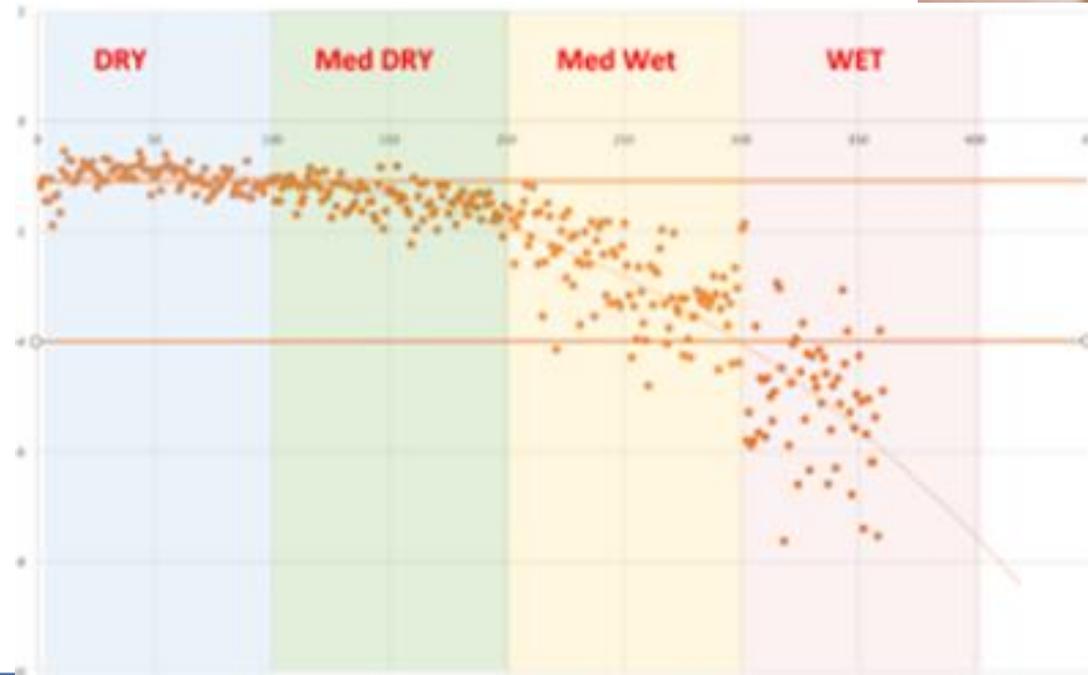
- UV-VIS Analysis of Medical Glass Tubes
- Medical device manufacturer using a new process
- Causing glass browning → Needs to be caught early



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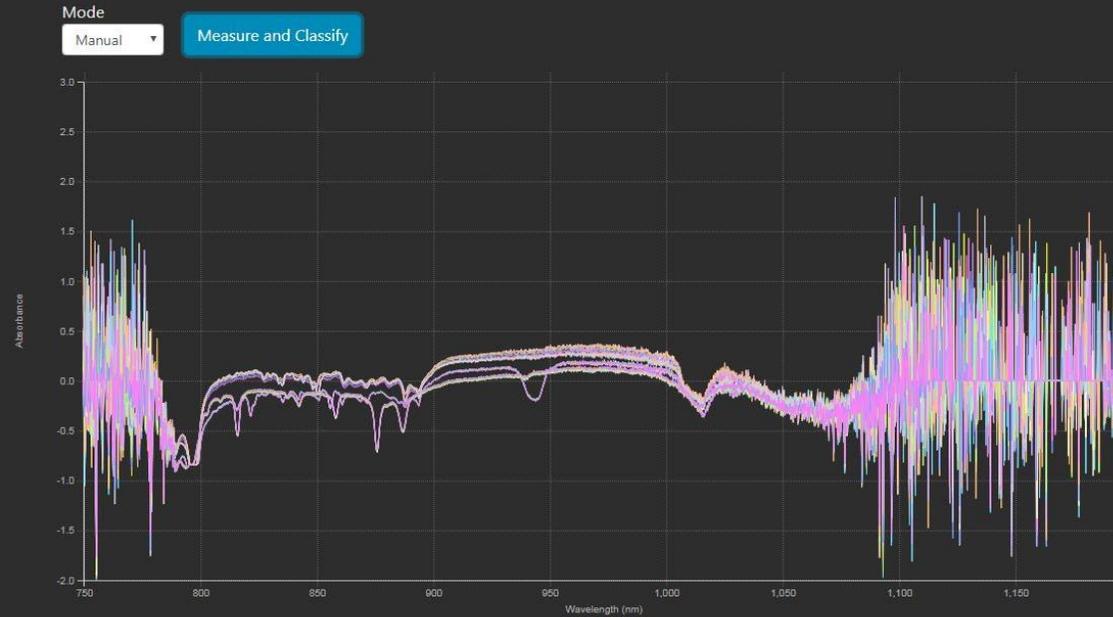
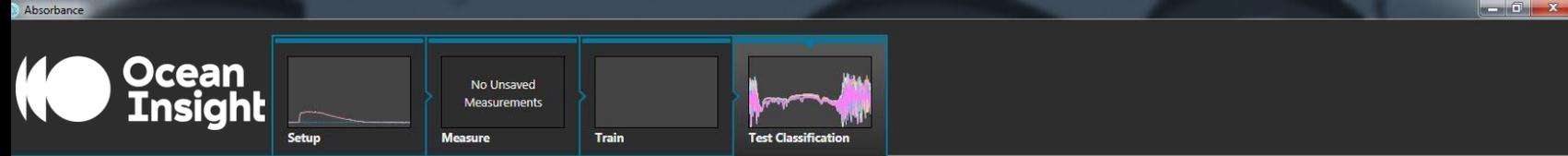
Applications in Spectral Machine Learning

- Food / Ag: Improving the process of sorting dates
 - Can neither be too dry or to moist!
- Rapid NIR Moisture Detection
 - 200ms/scan
- Fruit Binned by Automation
 - 4 Moisture Grades



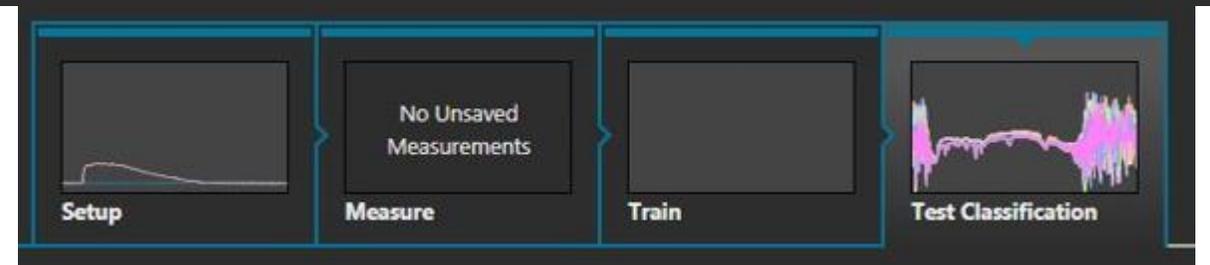
Applications in Spectral Machine Learning

- *Looping back to...*
- Raman Detection of Common Pesticides
 - <500ms Identification
 - High Confidence
- LSERS Technology



Classified Measurements

Measurement	Classification	Confidence
<input checked="" type="checkbox"/> Transmittance Scope		
<input checked="" type="checkbox"/> Measurement 1	Acetamiprid (82.9%)	
<input checked="" type="checkbox"/> Measurement 2	Acetamiprid (82.4%)	
<input checked="" type="checkbox"/> Measurement 3	Acetamiprid (78%)	
<input checked="" type="checkbox"/> Measurement 4	Phosalone (86.9%)	
<input checked="" type="checkbox"/> Measurement 5	Phosalone (78.8%)	
<input checked="" type="checkbox"/> Measurement 6	Phosalone (85.5%)	
<input checked="" type="checkbox"/> Measurement 7	Trichlorfon (70.1%)	
<input checked="" type="checkbox"/> Measurement 8	Trichlorfon (75.9%)	
<input checked="" type="checkbox"/> Measurement 9	Trichlorfon (71.1%)	
<input checked="" type="checkbox"/> Measurement 10	Thiram (84.6%)	
<input checked="" type="checkbox"/> Measurement 11	Thiram (85.6%)	
<input checked="" type="checkbox"/> Measurement 12	Thiram (90.7%)	
<input checked="" type="checkbox"/> Measurement 13	Acetamiprid (83.3%)	
<input checked="" type="checkbox"/> Measurement 14	Acetamiprid (77.9%)	
<input checked="" type="checkbox"/> Measurement 15	Acetamiprid (83.3%)	
<input checked="" type="checkbox"/> Measurement 16	Phosalone (76.7%)	
<input checked="" type="checkbox"/> Measurement 17	Phosalone (80.4%)	
<input checked="" type="checkbox"/> Measurement 18	Phosalone (81.2%)	
<input checked="" type="checkbox"/> Measurement 19	Trichlorfon (77%)	
<input checked="" type="checkbox"/> Measurement 20	Trichlorfon (79.4%)	
<input checked="" type="checkbox"/> Measurement 21	Trichlorfon (71.9%)	
<input checked="" type="checkbox"/> Measurement 22	Thiram (84.4%)	
<input checked="" type="checkbox"/> Measurement 23	Thiram (82.7%)	
<input checked="" type="checkbox"/> Measurement 24	Thiram (78.2%)	



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Expansions of Machine Learning

- Descartes Labs

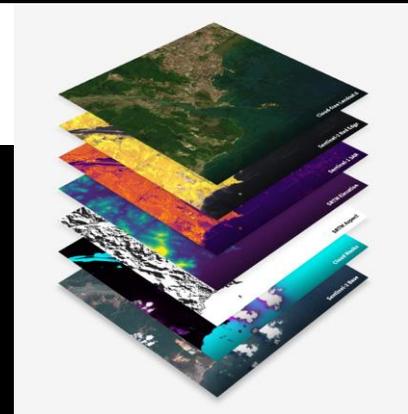
- *'A Data Refinery, Built To Understand Our Planet'*
- AI/ML Analyze Satellite/Map Data
- Understand Agriculture, Forestry, Water Cycles, etc to Help Business
- Field Boundaries / Crop Classification / Construction Trends

- Zebra Medical Vision

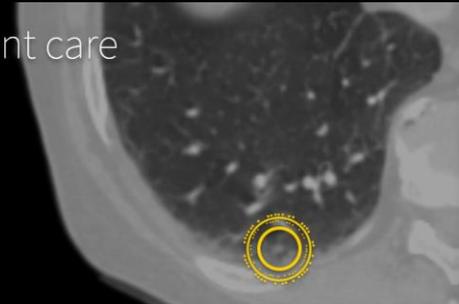
- *'Transforming Patient Care with the Power of A.I.'*
- AI/ML Analyze Radiology Scans
- Models Developed for Liver, Bone, Lungs, Heart

- Iris A.I.

- AI/ML search more accurately for scientific research papers
- Massive Database / Future Version to Auto-Create PPT's



Transforming patient care
with the power of



AI

Multispectral Imaging brought to wound care

- SpectralMD DeepView® wound imaging system
- Images blood flow deep in the tissue
- 90+% accurate in assessing burn depth and triaging patient wounds
- Experts: 70% accurate



- Machine learning algorithm detects tissue that can be saved and tissue that should be excised
- Reduces hospital stays and speeds healing

Recent feature in *Biophotonics*

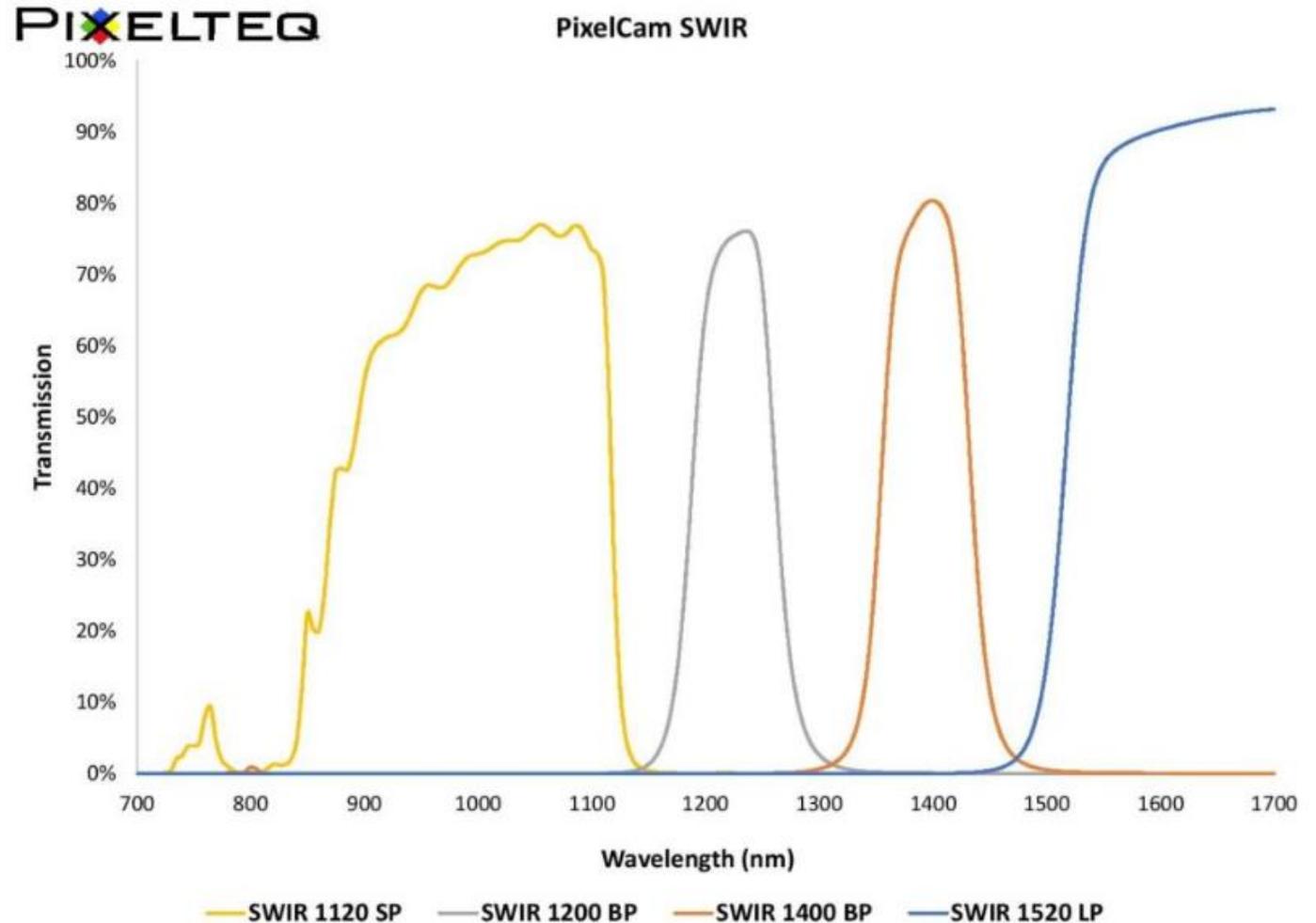
- Machine learning applied to multispectral imaging can reveal hidden features
- Speed advantage is key



Multispectral cameras are configurable

- Arbitrarily wide / narrow bands to fit particular applications
- Example – 4 band sensor
- Also 6, 9 band

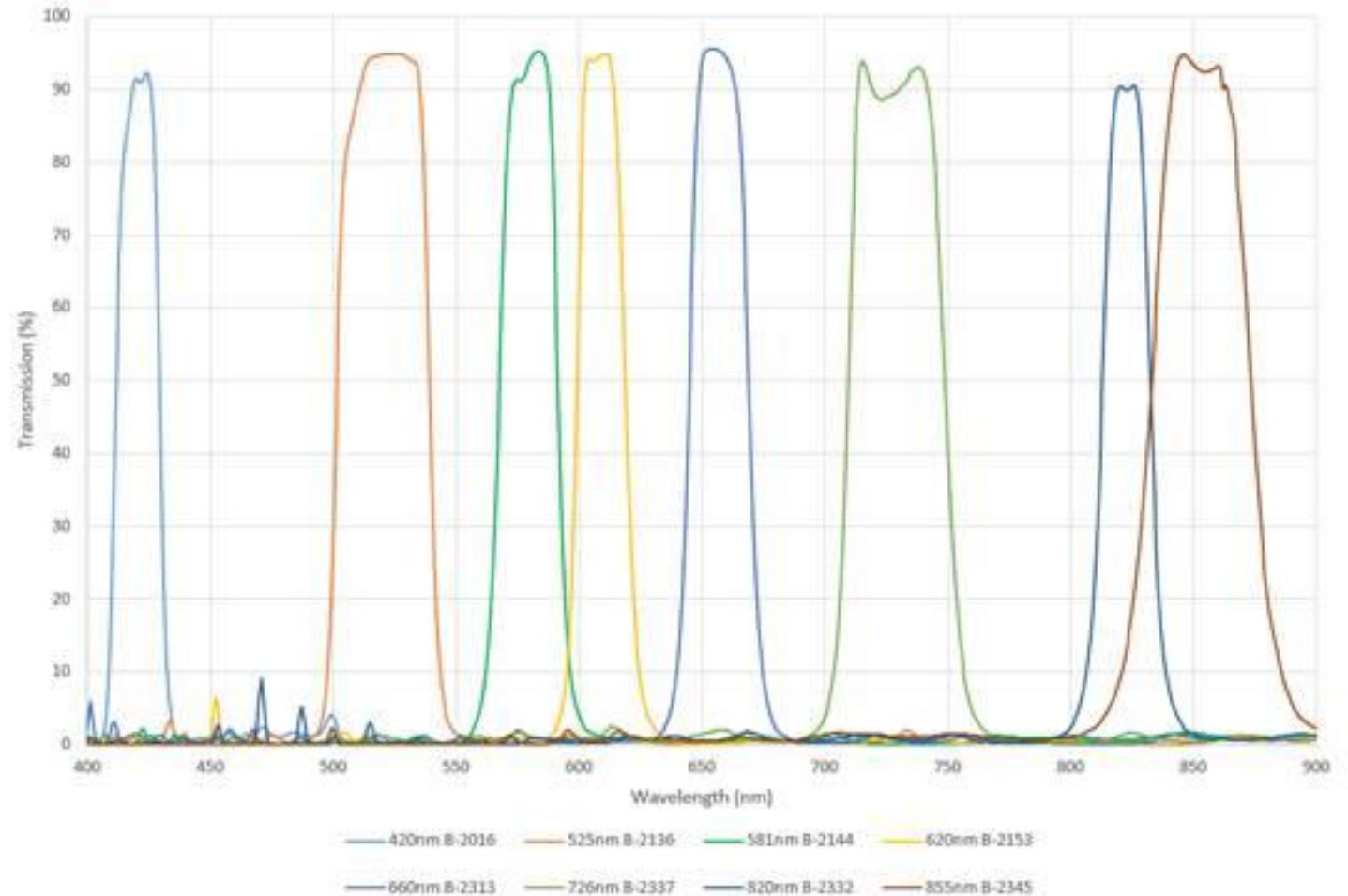
- Machine learning used to find optimal spectral bands
- Machine learning then used to process multispectral data



A visible multispectral camera

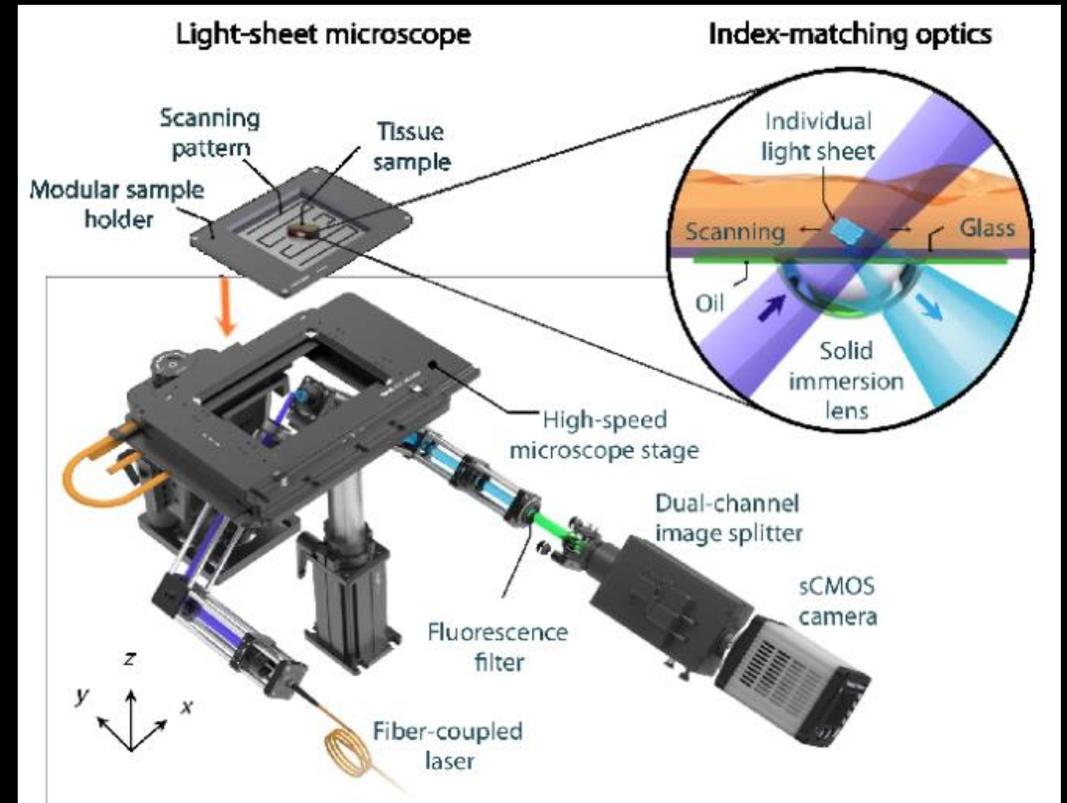
- Example of a 9-band system
- Advantage
 - Speed
 - Tailored to application
 - Inexpensive compared to hyperspectral imaging

PIXELTEQ



Application: Pathology

- Lightspeed Microscopy of Seattle is working on 3-D pathology instrumentation
- Novel light sheet microscope can reconstruct 3-D volumes of biopsies
- Computer image treatment and machine learning allow pathologists to visualize and find tumors



www.lightspeedmicro.com

Show the Lightspeed video here!

Lightspeed microscopy demo video.mp4

Thanks for joining us!

- Spectroscopy and Spectral Imaging will continue to accelerate our understanding in science and in business settings
- Machine Learning amplifies the understanding we can derive from spectral imaging tools

Come on the voyage with Ocean!



Unlock the Unknown