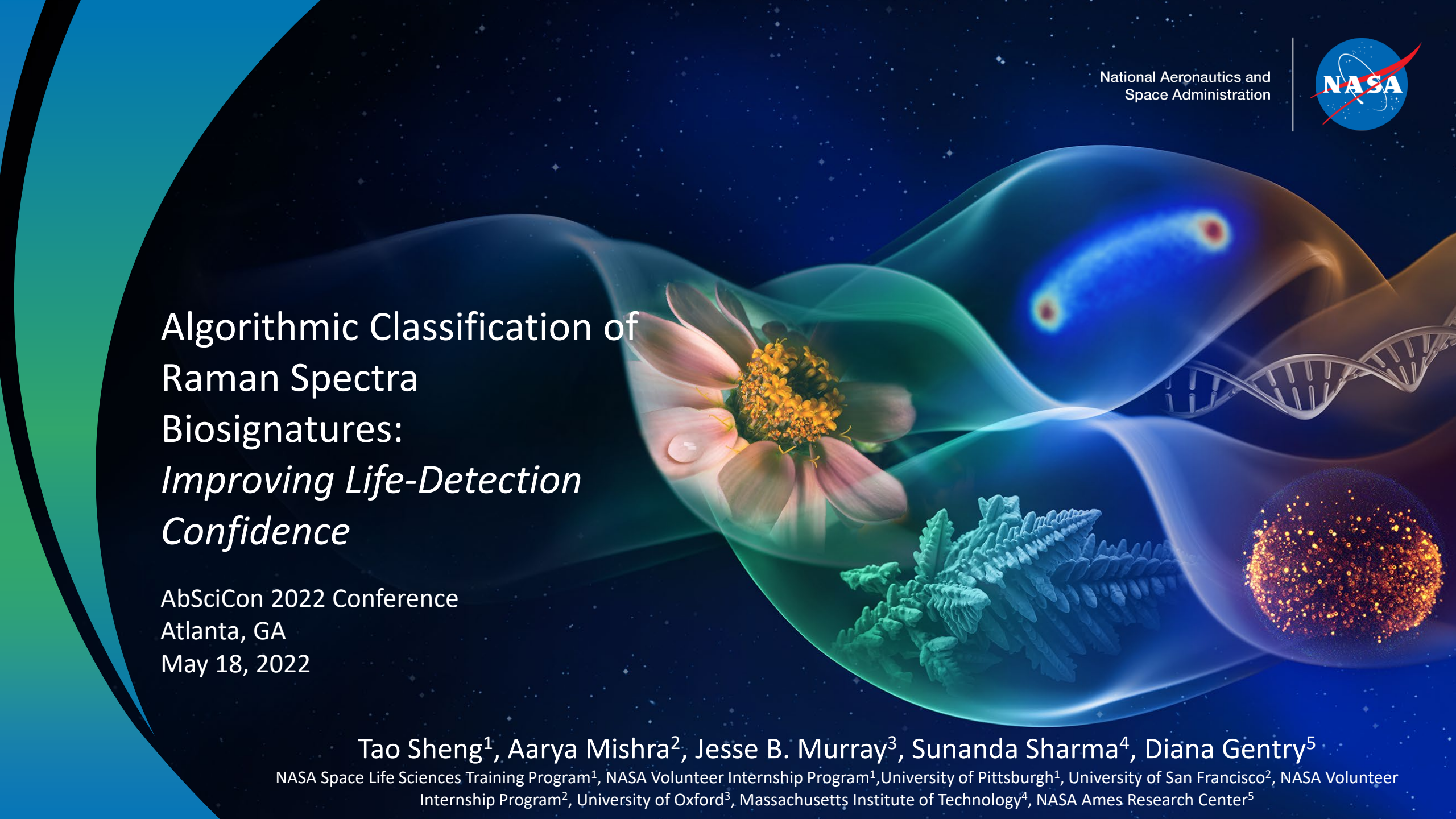
National Aeronautics and Space Administration



Algorithmic Classification of Raman Spectra Biosignatures: *Improving Life-Detection Confidence*

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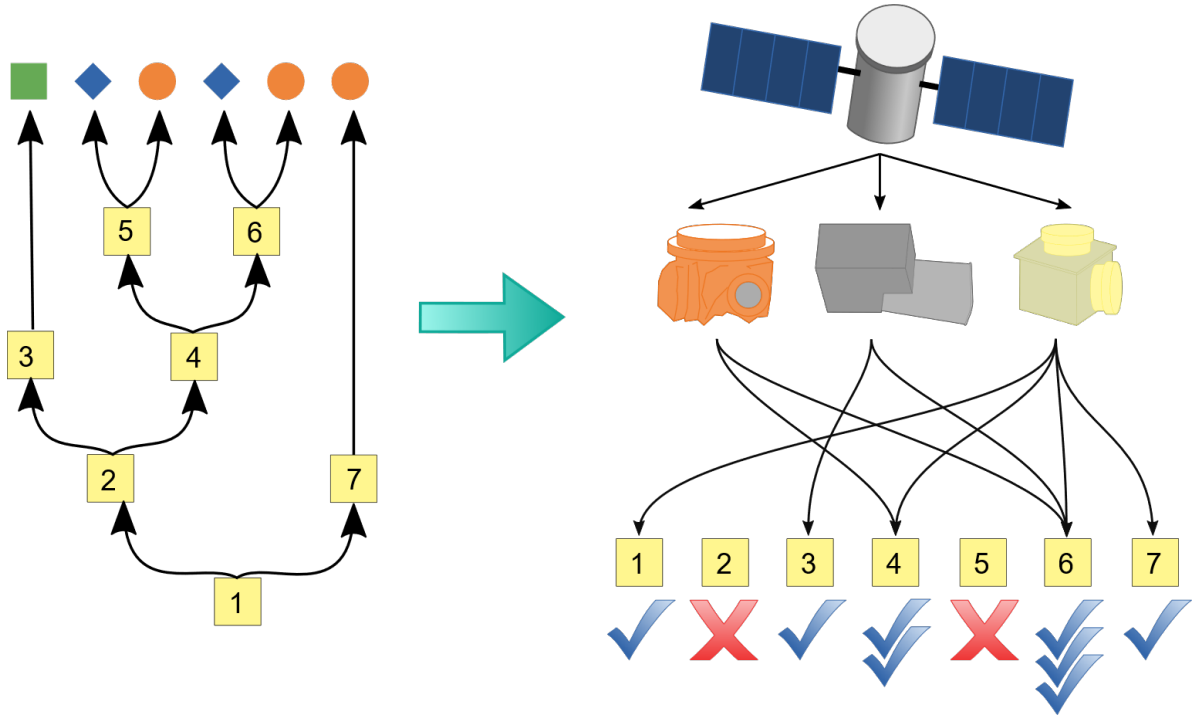
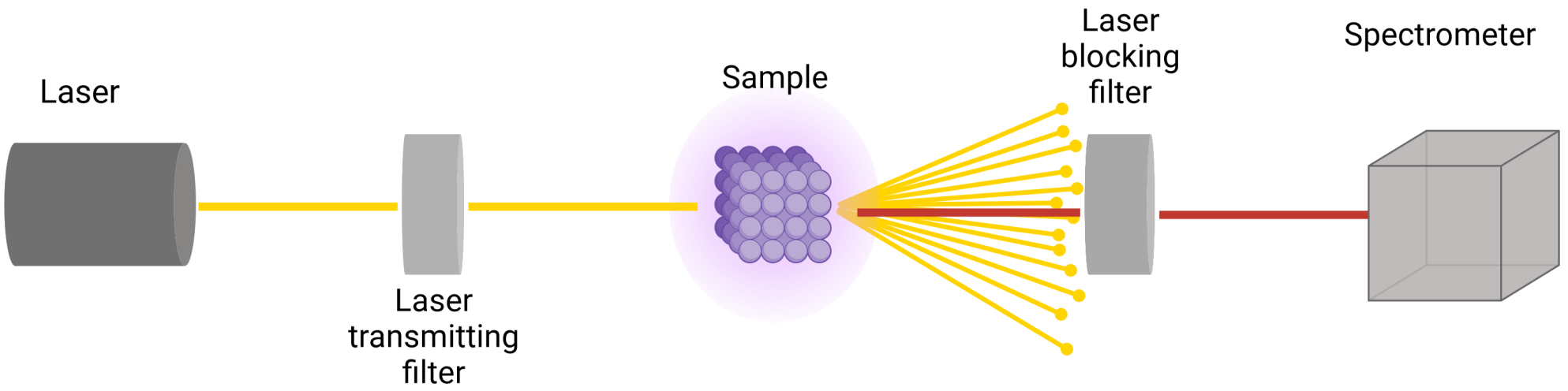
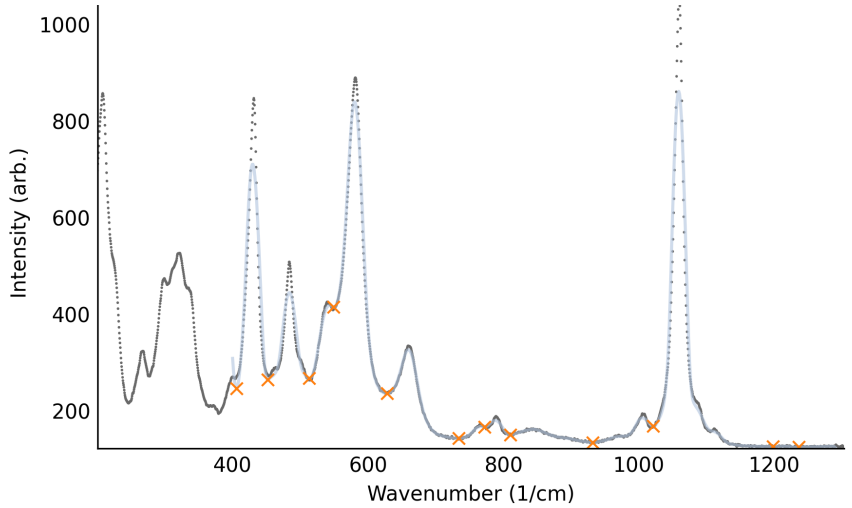
Background



Purpose: Algorithmically combine multiple, different instrument readings of the same potential biosignature to determine whether it is indicative or not indicative of life.

Raman Spectroscopy Basics





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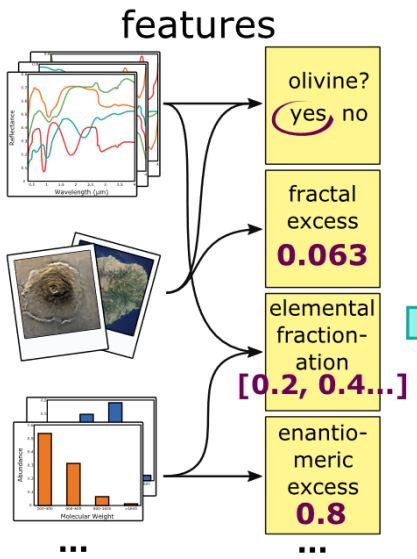
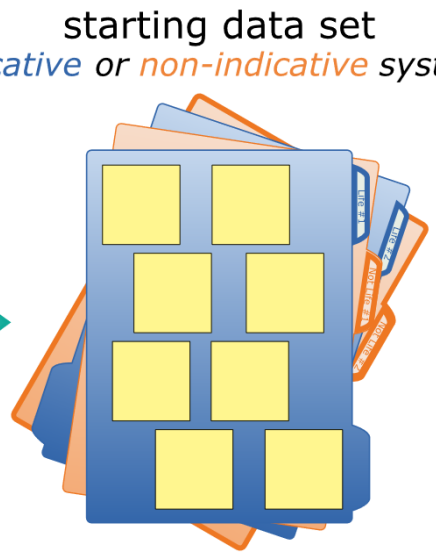
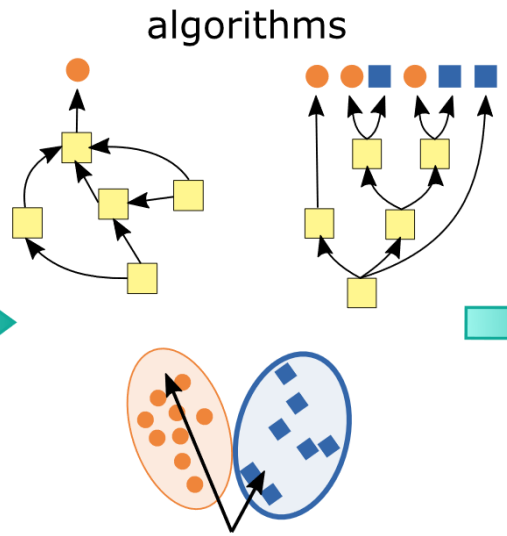
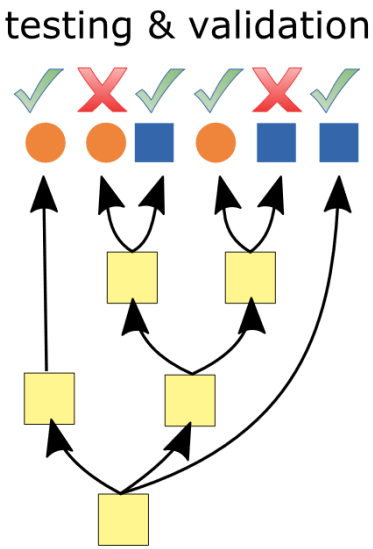
Overall Project Workflow









- Elemental abundance
- Isotopic fractionation
- VNIR reflectance spectra

- Collecting data on various materials

- Feature engineering
- Supervised learning

- Calculate accuracy, confidence, etc.

1) Data Selection

- **Previous data types:**
  - Elemental abundances, isotopic fractionation, visible and near infrared spectroscopy (VNIR)
- **Conditions**
  - Data collection feasibility in the field
  - Somewhat agnostic
    - Data type should not presuppose any specific biochemistry or molecular framework
      - Ex: Rover looking specifically for chlorophyll would not be agnostic
      - Ex: Rover looking for molecules that stores energy that ends up including ATP could be agnostic
    - Would be “putting the answer in the question”
  - Note on elemental abundance: the dataset is not perfectly agnostic because information on C, H, O, etc. allows bias towards C and water-based life
    - A more agnostic approach was taken to look at elemental distributions; this method no longer depends on C-based life and high amounts of water

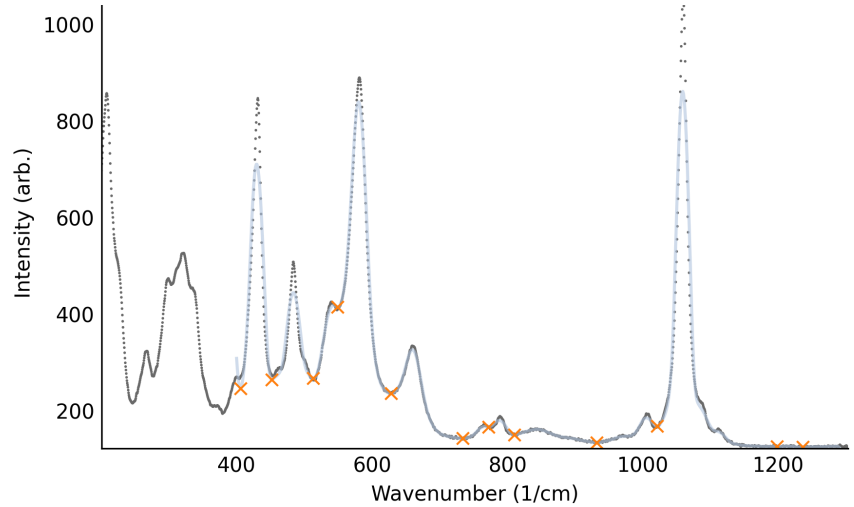
2) Data Collection

- **Curated indicative vs. non-indicative dataset**
  - – Distinctions unambiguous
  - – No edge cases (prions, etc.)
  - – Does not require an *a priori* definition of life
- **Raman data collection**
  - – Assembled from individual research articles and public domain databases
  - – "Standardized" to similar excitation lines (532nm or 514.5nm)
  - – Pre-processing: Savitzsky-Golay smoothing + interpolation, Polyfit baseline correction, Standard normal variate normalization

Class (subclass)	Class Definition	Examples
Indicative (alive)	Indicative sample of only alive materials	Vegetation, microorganisms, biofilm
Indicative (non-alive)	Indicative sample of only not-alive samples	Coral skeletons, coal, calcite
Indicative (mixed)	Indicative samples mixed with non-indicative	Non-sterilized silt, clay, or seawater
Non-indicative	Not alive and not indicative of life	Pure basalt, sand, or carbonatite

3) Feature Engineering & Algorithm Implementation

- **Feature engineering**
  - – Inaccurate feature engineering = inaccurate classifier
- **How can we describe spectral / Raman data agnostically?**
  - – Preliminary features: highest/lowest intensity, range, mean intensity, min/max 1st/2nd derivatives, # of peaks, # of troughs, broadest peak, mean peak width
- **Automated feature engineering**
  - – Image classification promising technique
- **Supervised learning**
  - – K-nearest Neighbors (KNN), Logistic Regression (LR) with L2 regularization, Support Vector Machines (SVM) with principal component, Gaussian Naïve Bayes (GNB), Random Forest (RF), Mean Votes

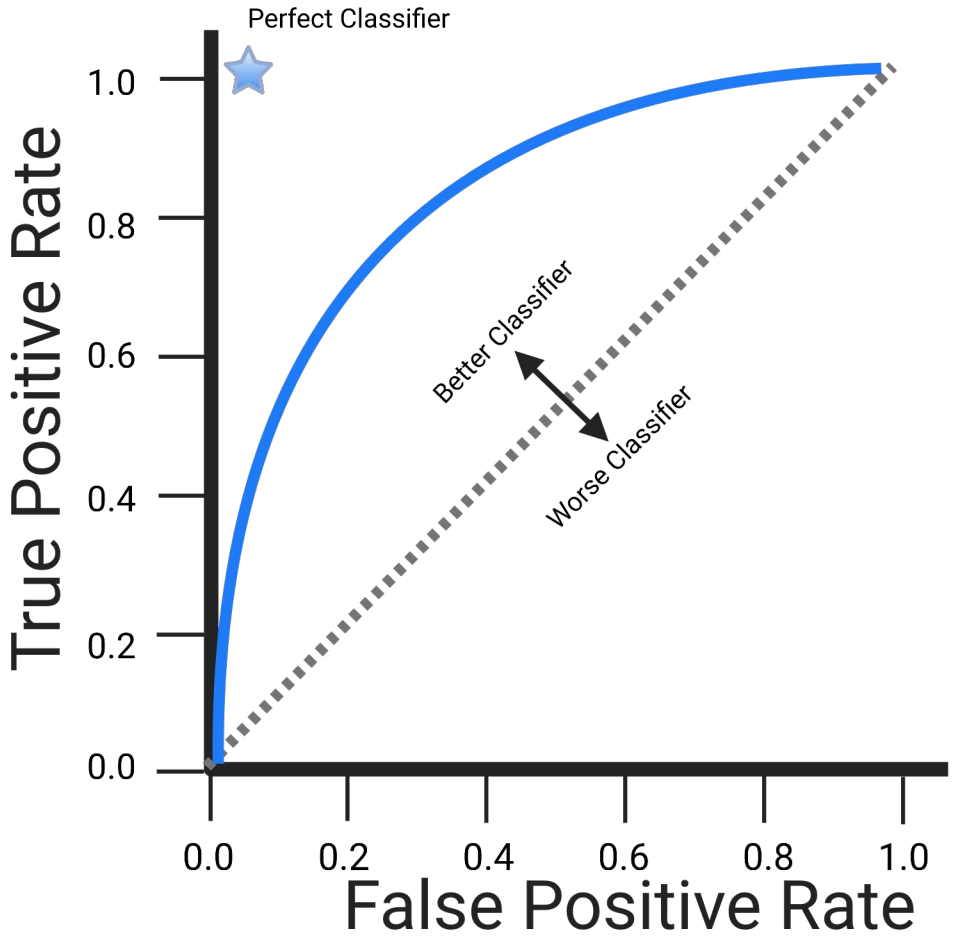


Example Raman Spectra of Hydroxyapophyllite, troughs detected as orange X marks

4) Testing Metrics & Validation

- **Accuracy metrics**
  - AUC: area under receiver operating curve (ROC)
    - Probability of correct classification
  - Done with 2,000 50% train-test-splits
- **False negative and false positive rates (FNR, FPR)**
  - Important in mission contexts where algorithm is deciding which samples to prioritize to evaluate further – erring towards more inclusion could be better
    - Indicated by slightly higher FPR than FNR

Sample Receiver Operating Curve (ROC)



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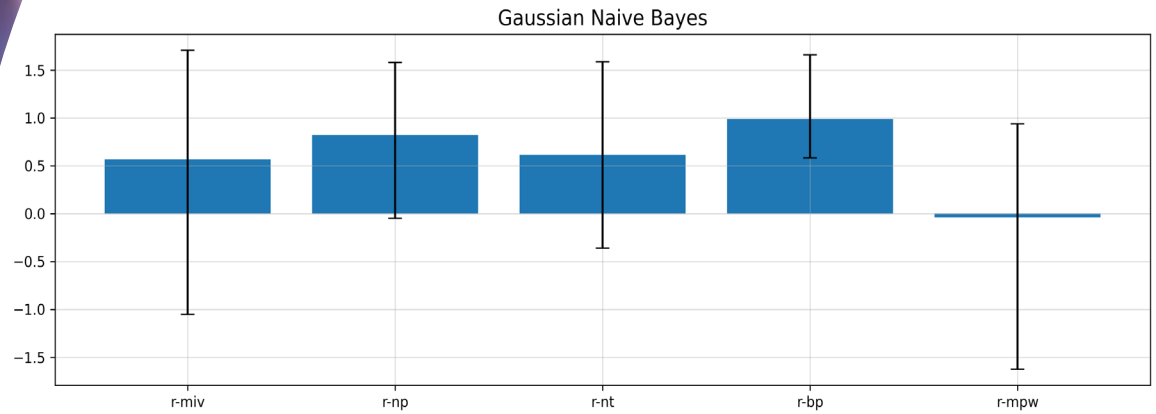
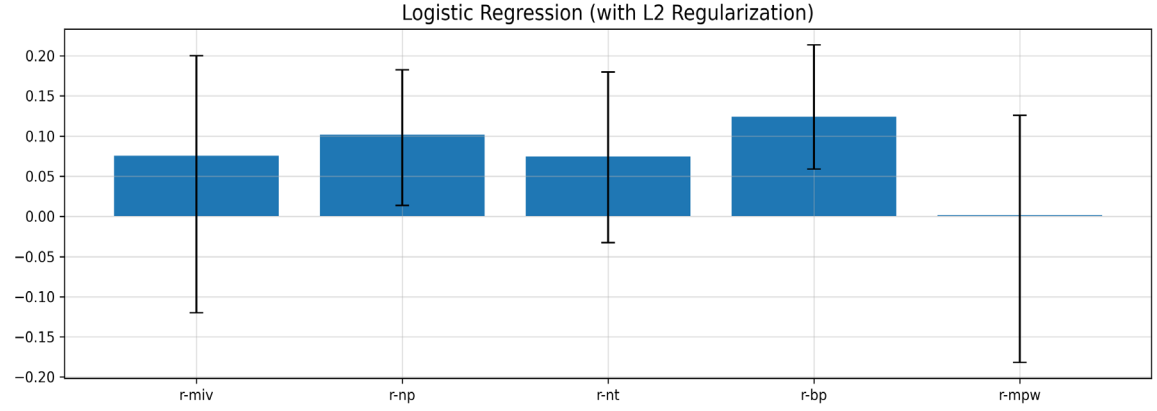
Raman Only Performance

Algorithms	*Raman Only*	*Raman Only, no mixed samples*
K-nearest neighbors (KNN)	0.772	0.789
Logistic regression (LR)	0.556	0.684
Support vector machine (SVM)	0.522	0.635
Gaussian naïve Bayes (GNB)	0.766	0.795
Random Forest (RF)	0.770	0.814
Mean voting performance (avg.)	0.808	0.860

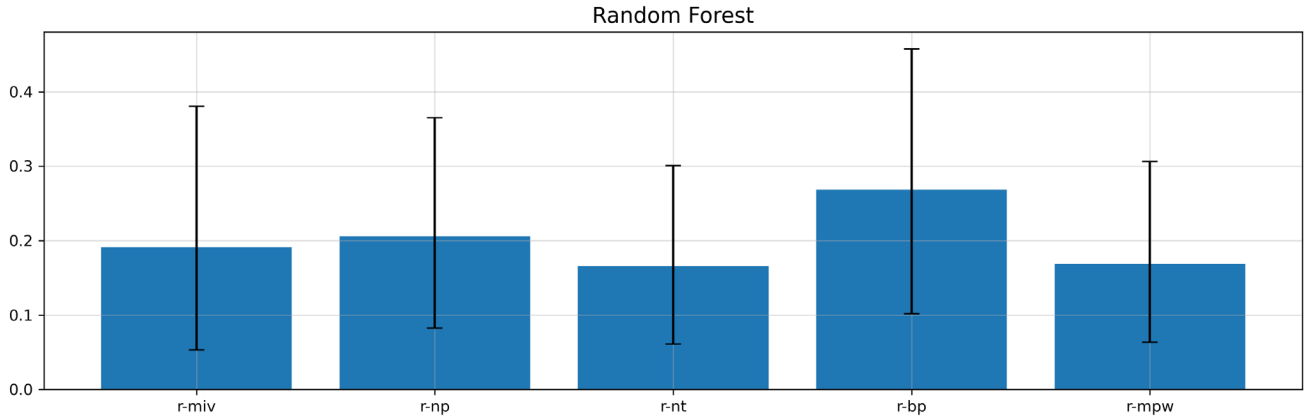
Feature Importance: Raman Data

Coefficients Feature Importance



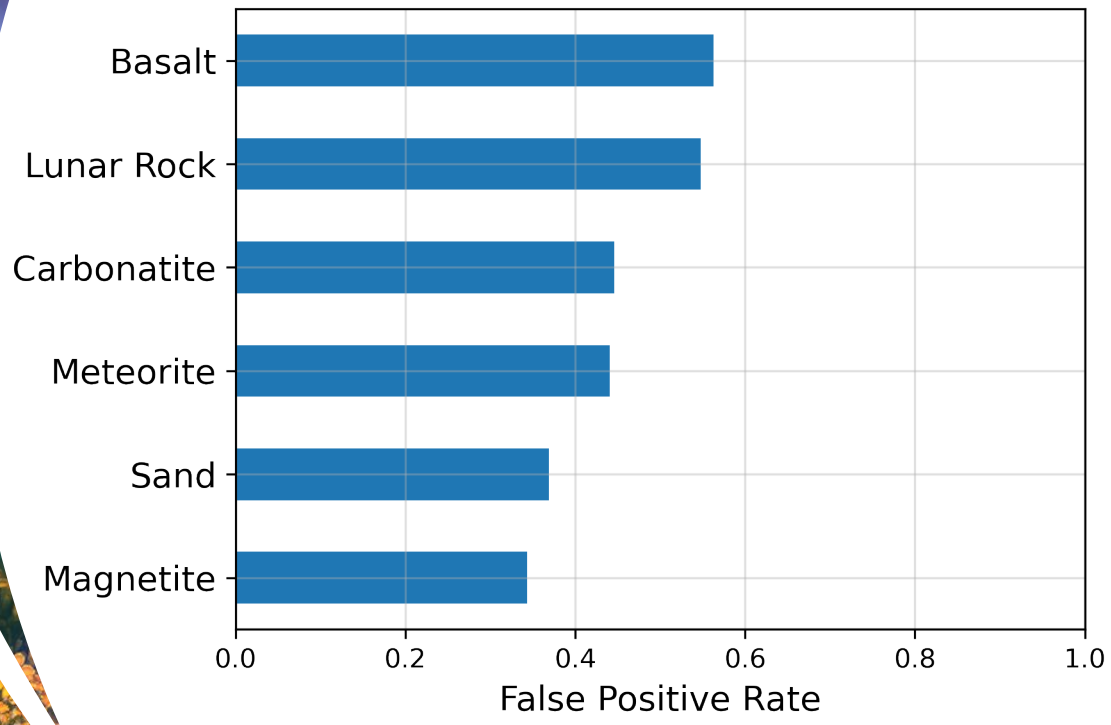


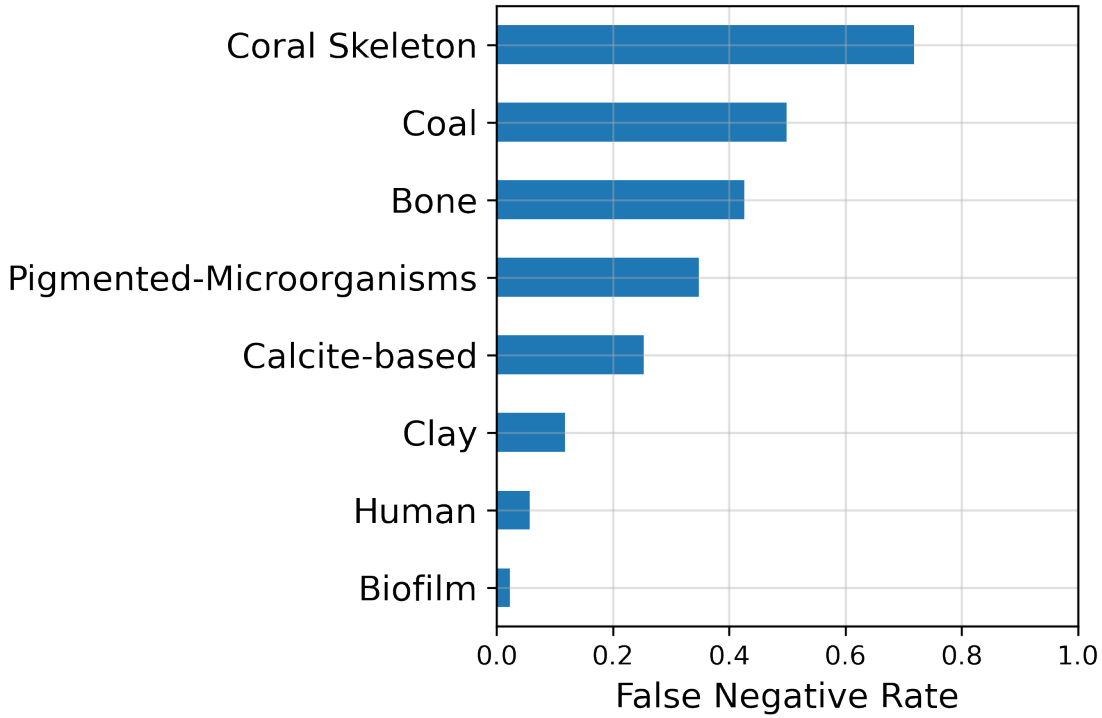
Decision Trees Feature Importance



Raman Common Misclassifications

- **Systems are disproportionally misclassified if they are indicative "mixed" or indicative not-alive**
  - Algorithm can more effectively classify between living vs. not living, but not so much when non-alive biosignatures are involved



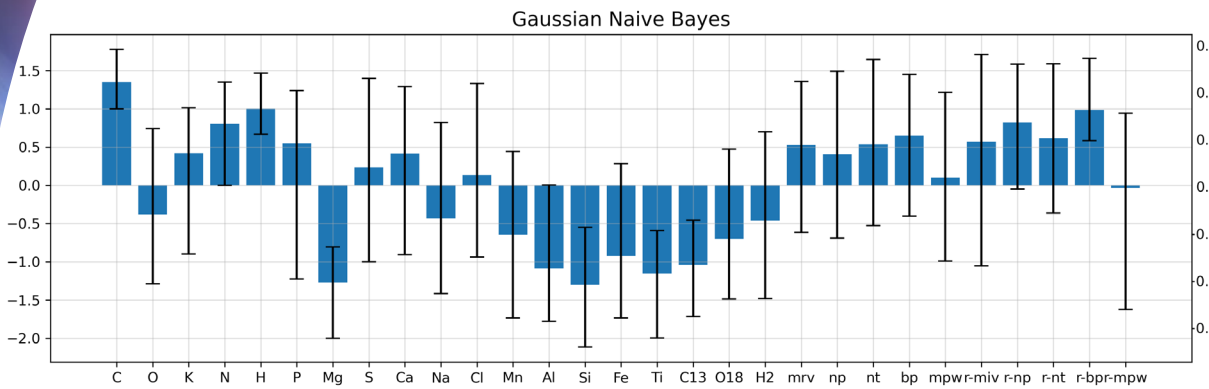


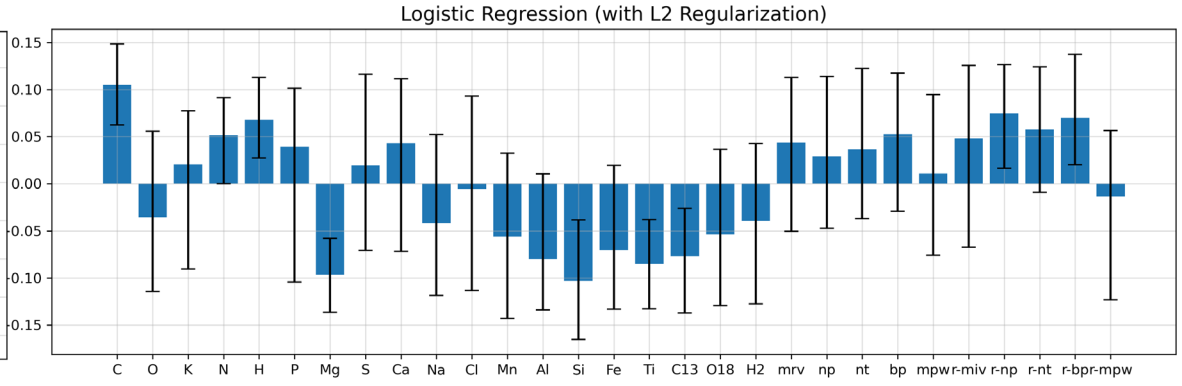
Combination Classification Performance

Algorithms	*Raman Only*	*Combination (Element, Isotope, Reflectance, Raman)*	*Combination (Element, Isotope, Reflectance, Raman) without mixed samples*
K-nearest neighbors (KNN)	0.772	0.759	0.798
Logistic regression (LR)	0.556	0.743	0.783
Support vector machine (SVM)	0.522	0.652	0.717
Gaussian naïve Bayes (GNB)	0.766	0.693	0.714
Random Forest (RF)	0.770	0.856	0.891
Mean voting performance (avg.)	**0.808**	**0.826**	**0.855**

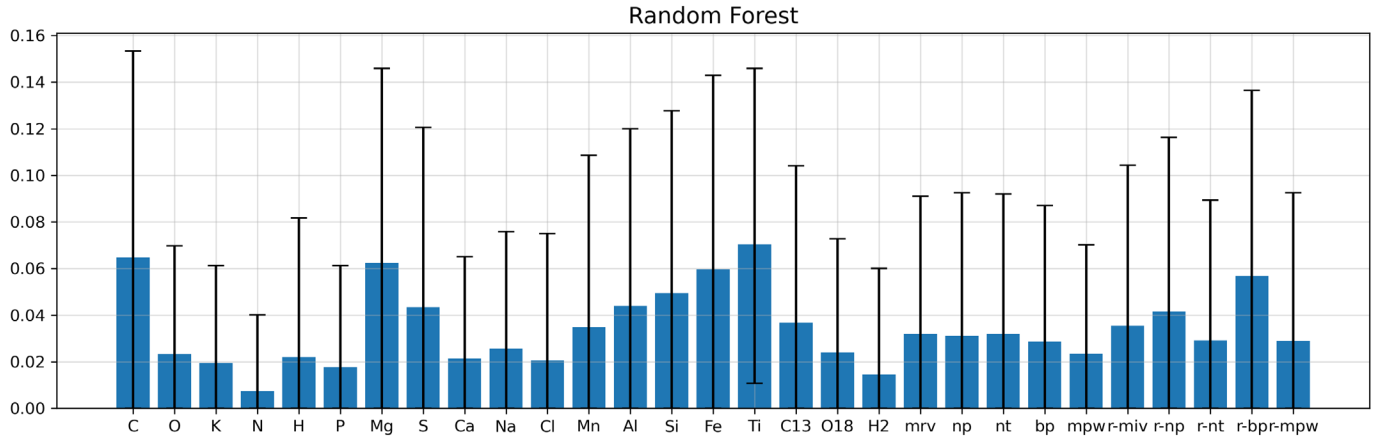
Feature Importance: Combined Data

Coefficients Feature Importance



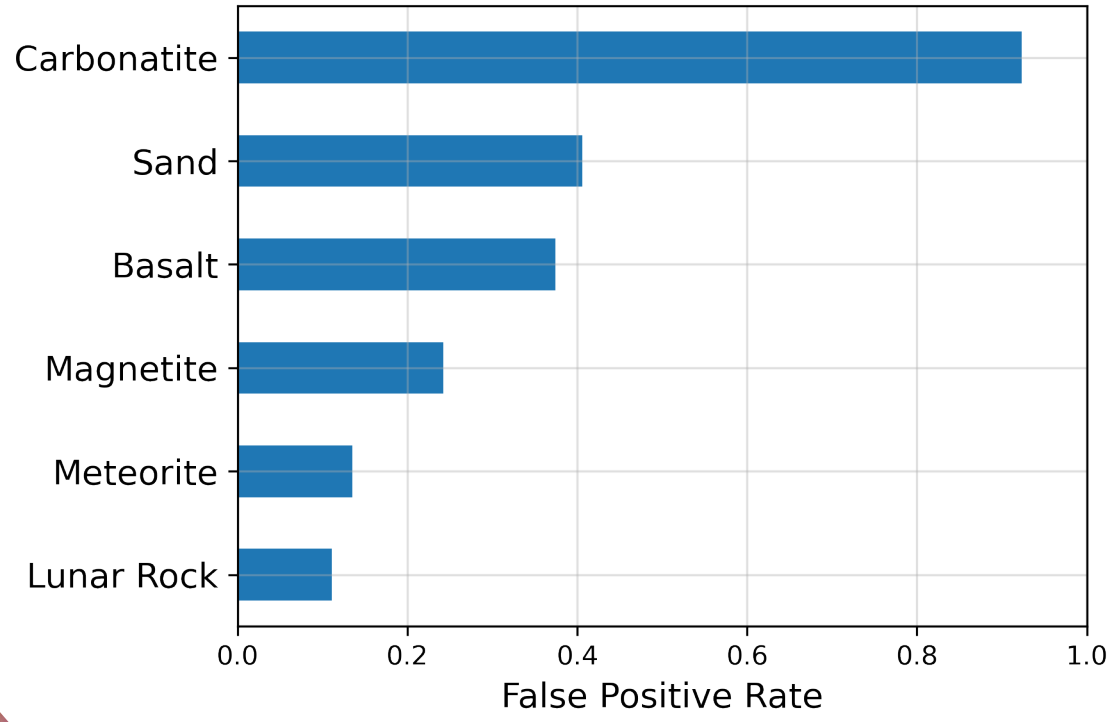


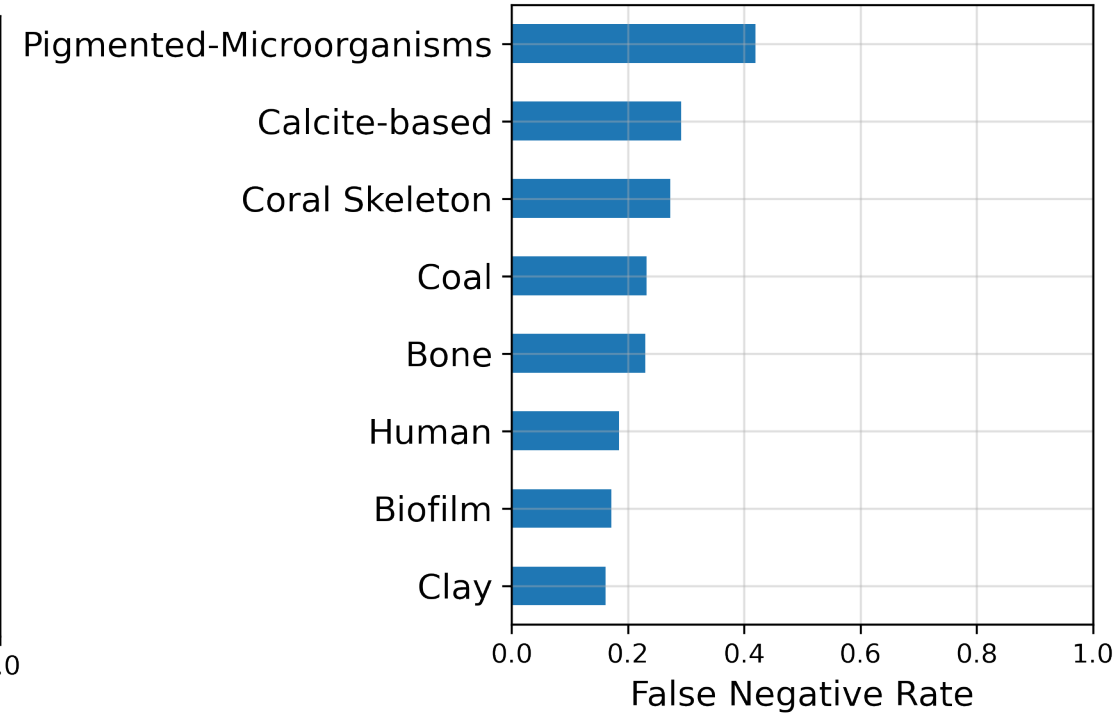
Decision Trees Feature Importance



Combined Common Misclassifications

- **Systems are disproportionally misclassified if they are indicative "mixed" or indicative not-alive**
  - Algorithm can more effectively classify between living vs. not living, but not so much when non-alive biosignatures are involved





Conclusions & Future Directions

- **Conclusions**
  - Manually engineered Raman features not very discriminatory, suggests need for other feature methods
    - Combined features rely heavily on C and H based life and ^{13}C delta ratio
  - Raman alone and combined performance improves without indicative-mixed samples
    - Mixed samples are more challenging to classify indicative alive or non indicative which suggests these supervised algorithms are better at life-detection but not so much with not-alive biosignatures
- **Future steps**
  - Image classification – automating feature extraction and improving VNIR reflectance and Raman classification
  - Further data collection of more “indicative / indicative mixed” raw Raman sample data
  - Further agnosticization with elemental abundance data to elemental distributions
  - Investigation into commonly misclassified systems

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Questions?

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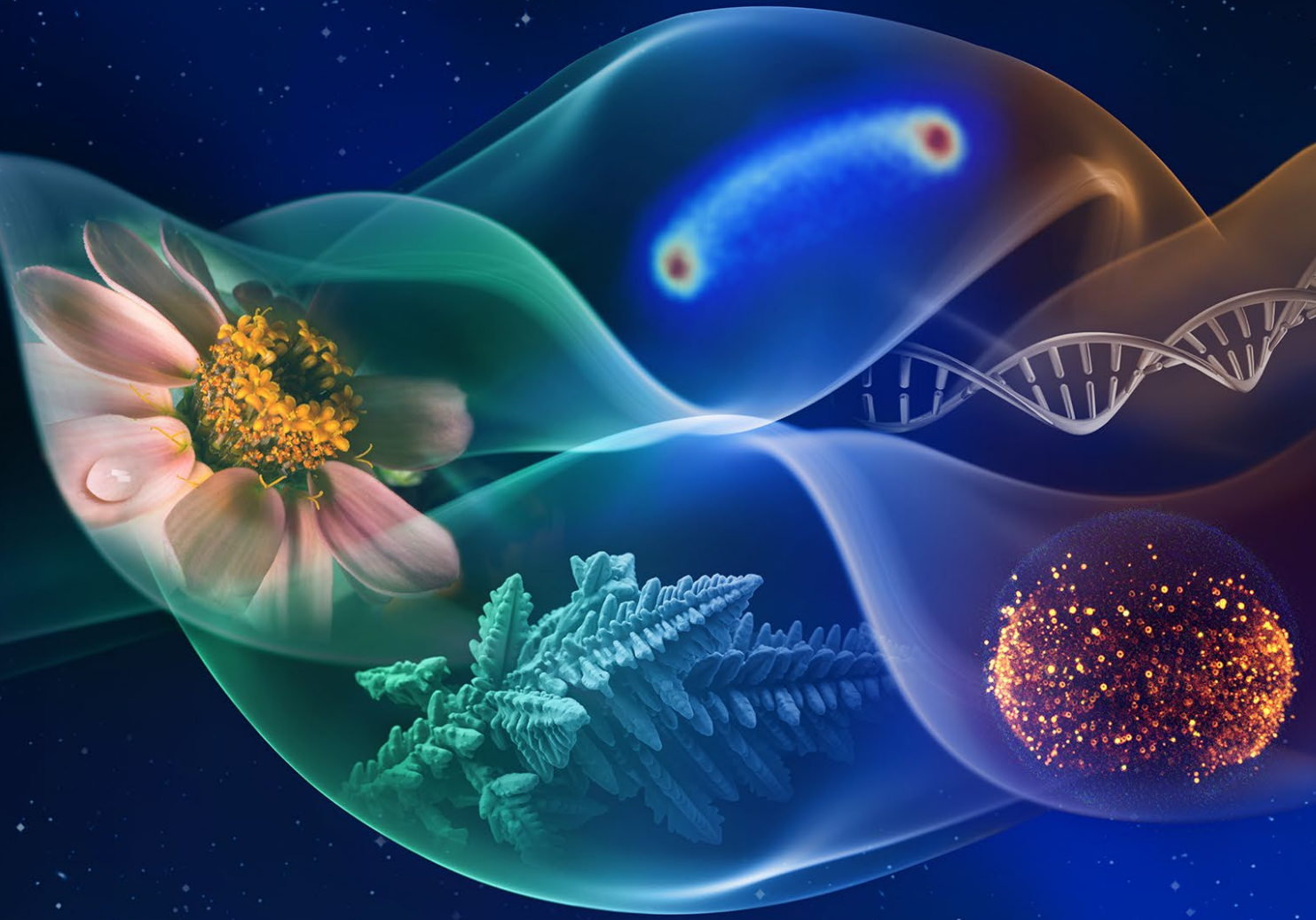

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