Summary and resources from the **Online Workshop: Databases and Software Tools for (FT)-IR Spectra for Microplastic Analysis**

03.06.25

The workshop was hosted by the joint collaboration between Norman Network, PlasticTrace, EAWAG and NIVA. This summary includes resources and publications shared during the workshop, and all presentations delivered during the workshop.

We welcome your feedback and suggestions for topics to include in future workshops—please don't hesitate to get in touch with us:

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Vilde Kloster Snekkevik: vilde.snekkevik@niva.no

Resources which were shared during the discussions:

For the Dutch monitoring of microplastics in marine sediments, developed in close cooperation with and performed by the NIVA laboratory, we have developed an R package, siMPleR, in cooperation with Wageningen University (NL). This package aggregates individual siMPle result files, performs basic QC on these files, performs basic data analyses and produces basic results tables and figures. A special feature of this package is that it integrates QC of a selection of microplastic records produced by siMPle using the Open Specy database, by adding the QC results in the siMPle import files.

Also note that Win Cowger has made it possible to directly import FTIR spectra, exported by siMPle, into Open Specy for an efficient quality control process.

We think that the combination of siMPle and Open Specy is a relatively simple and powerful combination for policy-oriented monitoring. However, other reference databases can of course also be used for external quality control.

The package is freeware and available from:

https://git.wur.nl/Walvo001/simpler

If you have any questions or comments about this package, please let us know.

With best regards,

Willem van Loon and Dennis Walvoort

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Dennis.walvoort@wur.nl

Agilent Whitepaper: https://www.agilent.com/cs/library/whitepaper/public/wp-microplastics-infrared-spectral-range-5994-8037en-agilent.pdf

JCGM Publications: Guides in Metrology:
https://www.bipm.org/en/committees/jc/jcgm/publications

Publications which were shared during the discussions:

- DOI 10.1016/j.talanta.2021.122624
- https://doi.org/10.1016/j.ecoenv.2024.116243
- https://pubs.acs.org/doi/10.1021/acs.est.4c09427
- DOI: 10.1016/j.scitotenv.2023.163612

Summary of the discussions based on the questions, answers and comments in the chat (AI generated):

For the quantification microplastics, setting clear limits of detection (LOD) and limits of quantification (LOQ) is essential. Measurements below the LOQ typically carry uncertainties greater than 30%, and when approaching the LOD, uncertainties can exceed 100%. This highlights a critical limitation: we often cannot identify smaller particles with confidence. As demonstrated in specific case examples, these uncertainties must be accepted and transparently reported. Any software used for microplastic analysis should include functionality to define and communicate these detection and quantification limits.

Filter selection also plays a key role in the quality of microplastic data. Currently, silver filters are emerging as a practical choice due to their affordability (approximately $2 per filter) and their flat, reflective surface. While options like silicone, Anodisc, or gold-coated polycarbonate offer superior analytical performance, they come at a significantly higher cost—around $20 per filter—creating a trade-off between budget and precision.

A common benchmark in microplastic studies is the collection of at least 100 particles per sample to ensure statistical representativeness. However, this threshold is not always attainable, especially in samples with low particle abundance or when processing is expensive. In light of this, some researchers are questioning whether we should move away from rigid particle count requirements. Modern, high-throughput, algorithm-driven workflows now offer the ability to rigorously quantify uncertainty, making it possible to shift the emphasis from arbitrary thresholds toward more meaningful, data-driven confidence estimates. For example, one lab reported an average 14% underestimation in particle counts and now provides detailed uncertainty metrics to collaborators, embracing this more flexible and transparent approach.

In terms of instrument settings, it's important to note that when using stainless steel mesh filters, the step size (or resolution) of the device should actually be larger than the mesh holes. This allows the instrument to "smooth over" the mesh structure rather than being disrupted by it. Additionally, spectral resolution constraints must be considered: while FTIR data can be downscaled to LDIR wavelengths, the reverse is not possible, requiring thoughtful planning in spectral analysis.

Measurement uncertainty remains a complex and often misunderstood topic in this field. Despite the formal definition provided by the International Vocabulary of Metrology (VIM), many still conflate general variability with true uncertainty. The latter should encompass all influencing factors—from sampling to instrumental limitations—and be estimated according to rigorous, standardized metrological procedures. At present, inconsistent terminology and approaches reflect the broader lack of harmonization in microplastic research. This gap underscores the need for collaborative standardization efforts and interlaboratory comparisons (ILCs), which can help establish the actual detection and quantification capabilities of current methodologies. As some experts suggest, we may currently be overestimating our analytical precision.

Another source of uncertainty stems from the environmental transformation of particles. Physical aging, chemical interactions, and surface coatings (such as biofilms, heavy metals, or

PAHs) can significantly alter a particle's FTIR spectral signature, increasing the risk of misidentification or false negatives. These issues call for the development of robust pre-processing or correction algorithms, as well as updated reference libraries that account for environmentally induced spectral distortions.

Ultimately, to ensure that microplastic data generated today remains meaningful and useful in the future, we need to develop tools and frameworks that allow for transparent, comparative, and standardized uncertainty assessment. This includes defining what level of uncertainty is acceptable for specific research or regulatory contexts—effectively answering the question: "how good is good enough?".

NORMAN

Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

Working Group N°4: Nano- and micro-scale particulate contaminants

Databases and Software Tools for (FT)-IR Spectra for Microplastic Analysis

Tuesday 3rd of June, 14:00 - 16:00 CEST

NORMAN Working Group N°4: Nano- and micro-scale particulate contaminants

Ralf Kägi (Eawag), Bert van Bavel (NIVA), Vilde Kloster Snekkevik (NIVA)

eawag aquatic research

NIVA

norman

PlasticTrace
Tracing Micro and NanoPlastics in Food and Environment

NORMAN
Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances

Working Group N°4: Nano- and micro-scale particulate contaminants

The NORMAN network on Chemicals of Emerging Concern

www.norman-network.net

norman

Network of reference laboratories, research centers and related organisations for monitoring of emerging environmental substances

- **Who is NORMAN:**
  - Non-profit association **since 2009** (former EU-funded project)
  - More than **90 members** from leading organisations in Europe, North America, Asia, Australia
- **Mission:**
  - Enhance **the exchange of information** and **collection of data** on emerging environmental substances
  - Improve **data quality**
    - Encourage the **validation** and **harmonisation** of common **measurement methods** and **monitoring tools** so that the demands of risk assessors can be better met
  - Promote **synergies** among research teams and more efficient **transfer** of research findings to policy-makers
- **Vision:**
  - **Independent**, transparent and open network working for a sustainable environment
  - **Bridge** between science and policy-making
  - Platform for **innovative** initiatives to address **contaminants of emerging concern** in the environment and new monitoring challenges

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Working Group N°4: Nano- and micro-scale particulate contaminants

NORMAN Working Groups

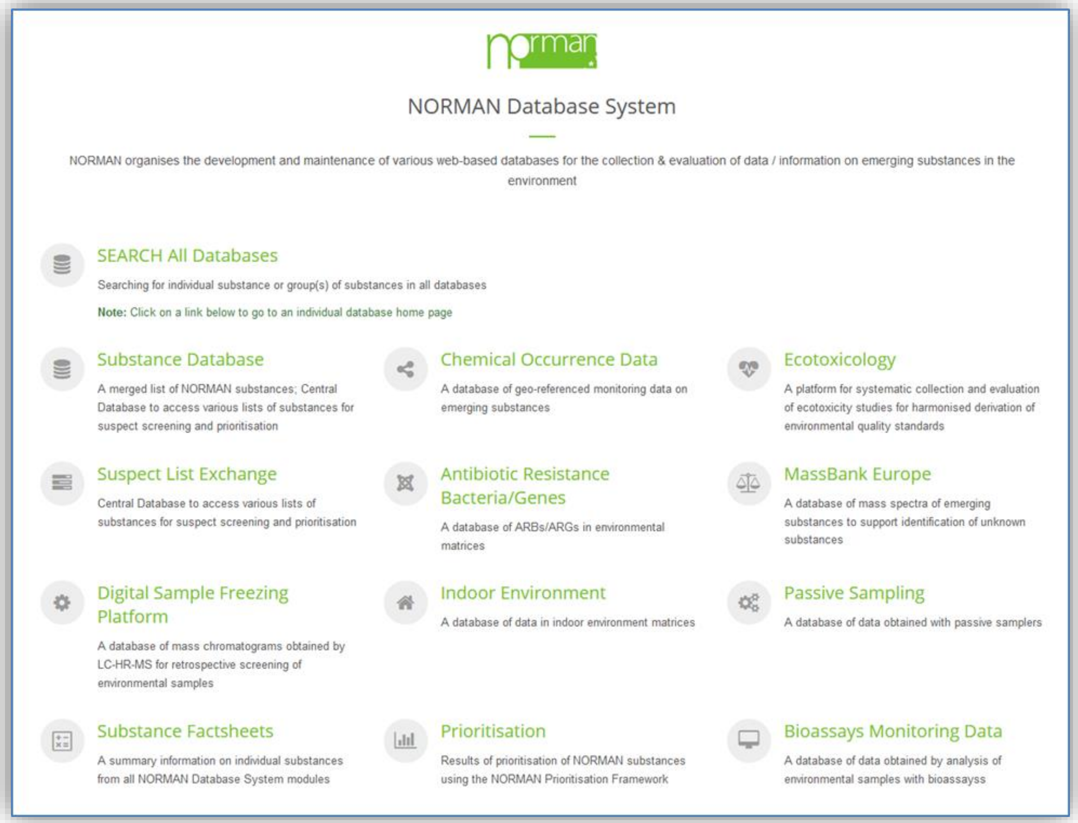
WG1: Prioritisation
WG2: Bioassays and biomarkers in water quality monitoring
WG3: Effect-directed analysis for hazardous pollutants identification
WG4: Nano-and micro scale particulate contaminants
WG5: Water reuse and policy support
WG6: Indoor environments and ambient air
WG7: Contaminants of emerging concern in soil and the terrestrial environment
WG8: Marine

Cross-Working Group Activity: Passive sampling
Cross-Working Group Activity: Non-target Screening (NTS)

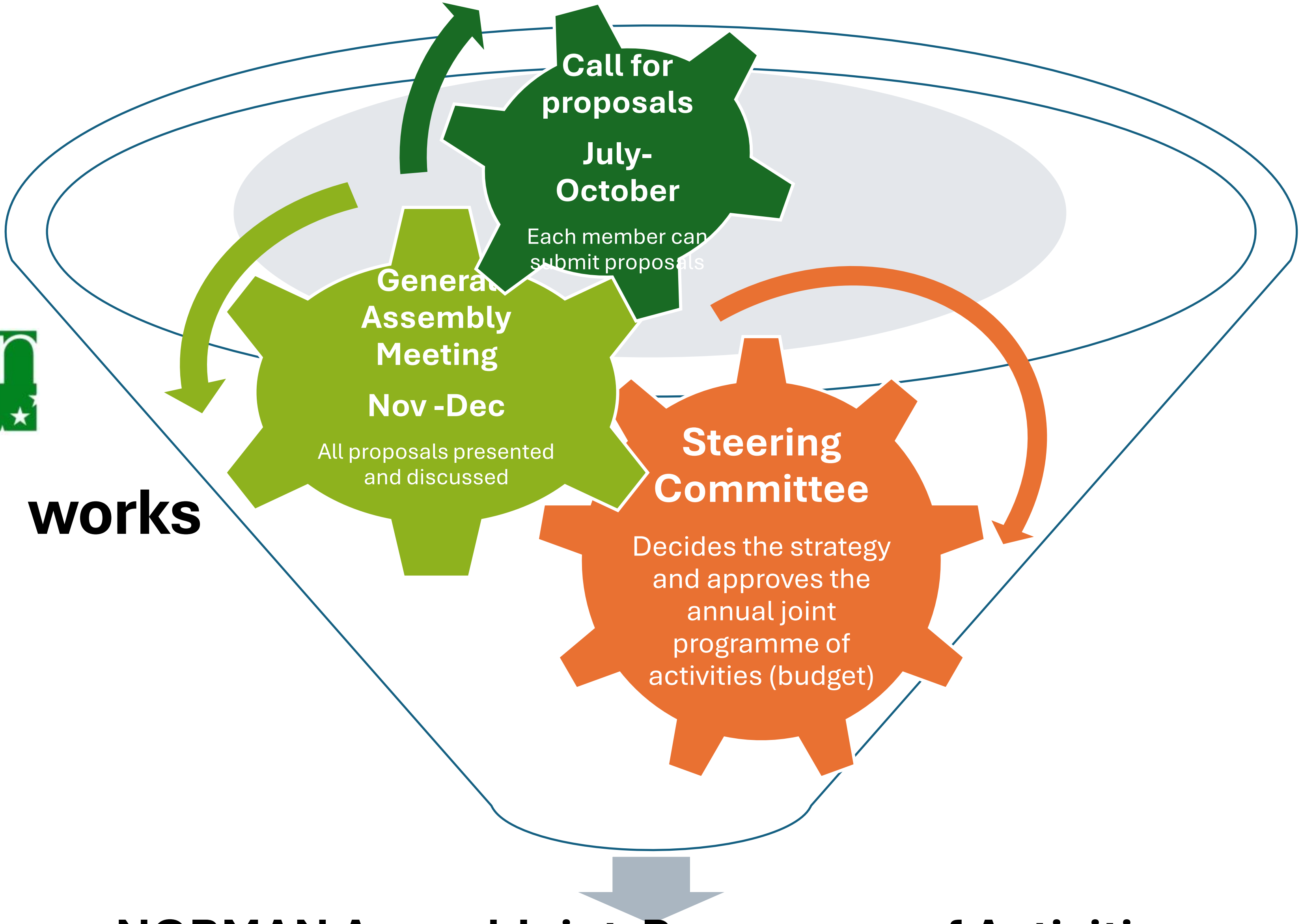
NORMAN Database System

NORMAN Database System

- **Open access** platform of interconnected databases (EMPODAT already synchronized with IPCHEM), implementing **FAIR** principles
- All modules **connected** via a **unique identifier**
- **Not only monitoring data**, but also substance properties, ecotoxicity data, info to support identification of unknowns in HRMS spectra
- **Harmonized** protocol for **data collection** and data **reporting**
- Paving the way for development of a new European infrastructure to handle data coming from **innovative methods** (e.g. NTS and effect-based methods) in line with the Green Deal objectives.



How NORMAN works



NORMAN Annual Joint Programme of Activities

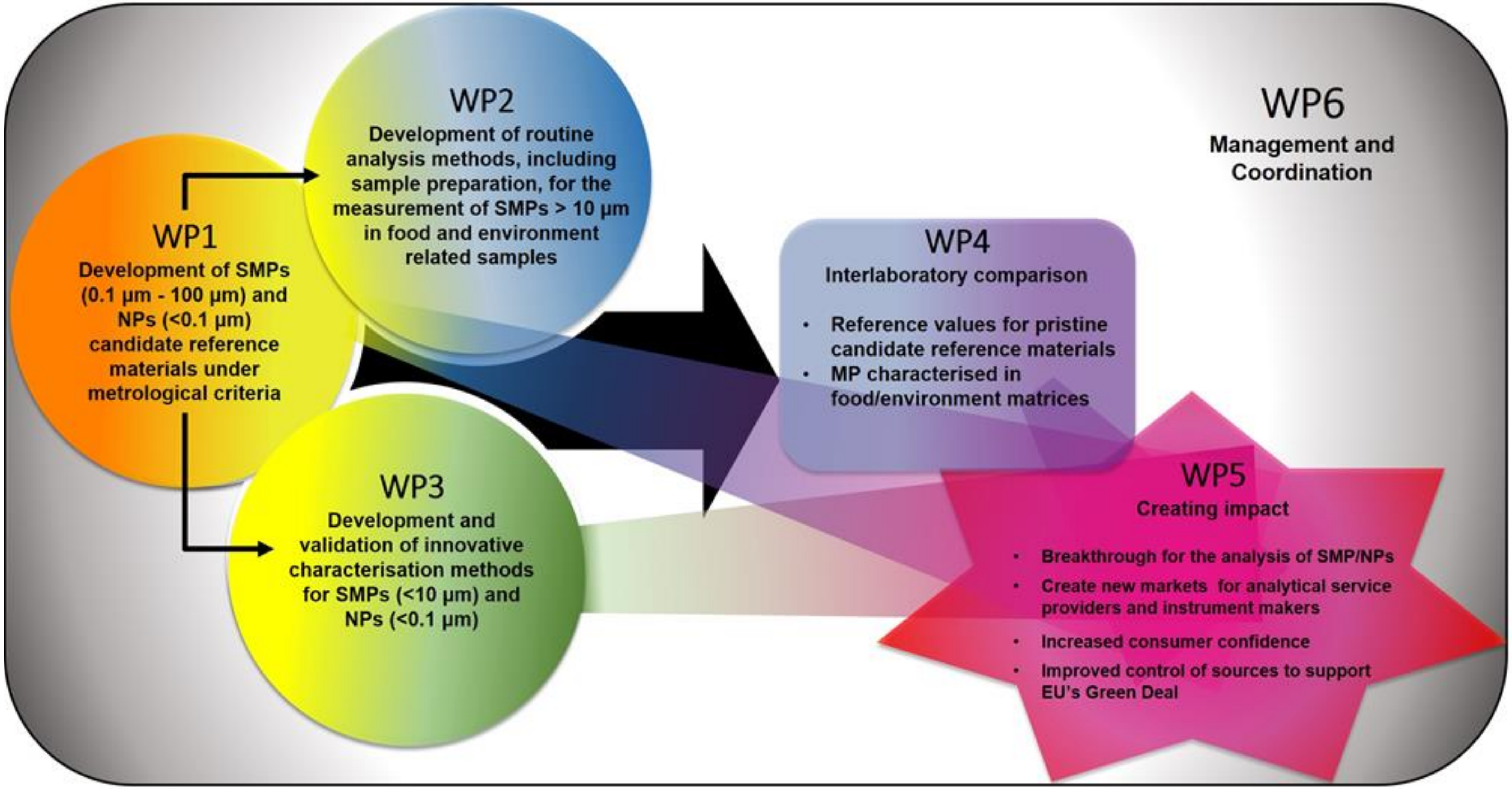
https://www.norman-network.net

Annual Report of Activities and Financial Report approved by ALL members

The Project – PlasticTrace

The overall aim of PlasticTrace is to **develop** international metrological capacity that enables the **traceable measurement** and characterisation of **small-micro plastics (SMPs; 100 – 0.1 µm)** and **nanoplastics (NPs; < 0.1 µm)** in environmental and food samples and the production of suitable **reference materials**, according to the metrological requirements.

Overview of PlasticTrace Work Plan



Working Group N°4: Nano- and micro-scale particulate contaminants

Jes Vollertsen, Aalborg University:
"The role of FTIR spectral databases and quantification algorithms for microplastic identification – exemplified by the siMPle freeware"

Benedikt Hufnagl, Hufnagl Chemometrics GmbH:
"Using AI and large-scale spectral databases for polymer identification of microplastics"

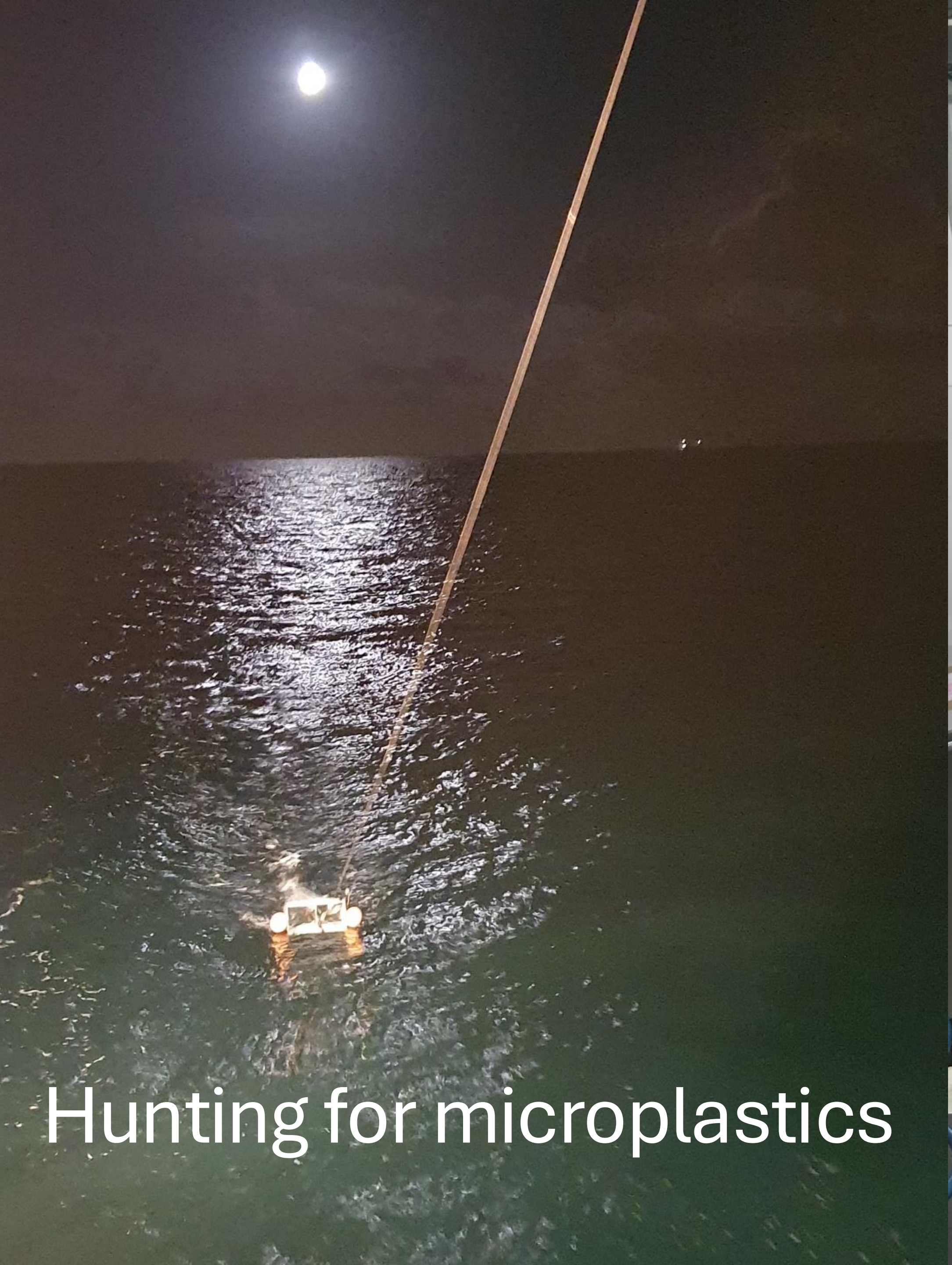
Eric Ceglie, Empa:
"Software developments for particle detection and quantification based on FT-IR hyperspectral data"

Win Cowger, Open Specy:
"Automated microplastic spectroscopy, biases, limitations, and opportunities"

“The role of FTIR spectral databases and quantification algorithms for microplastic identification – exemplified by the siMPle freeware

Jes Vollertsen

Professor of Environmental Engineering, Aalborg University, Denmark


Hunting for microplastics

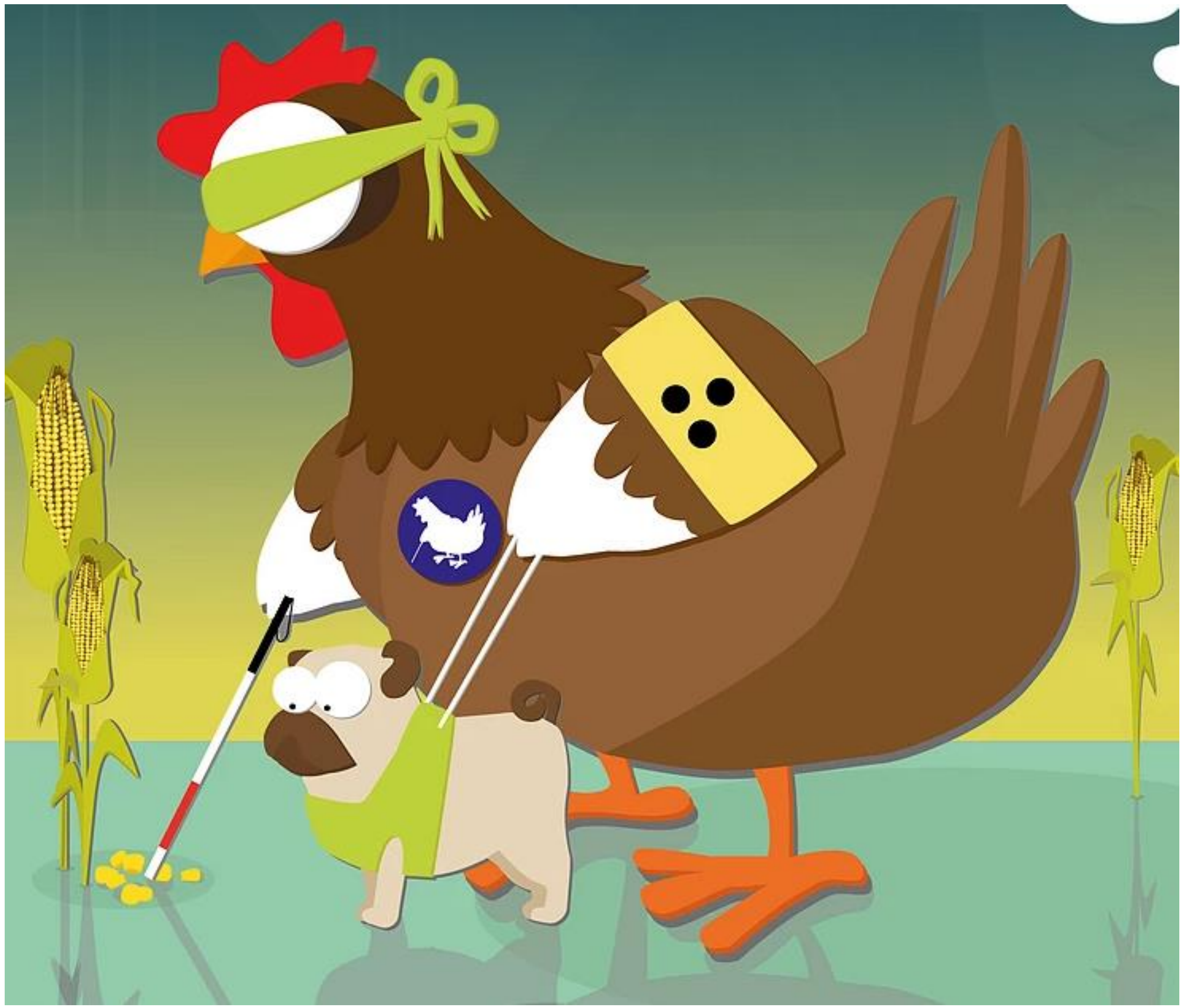

YES – we found one

But did we find them all?

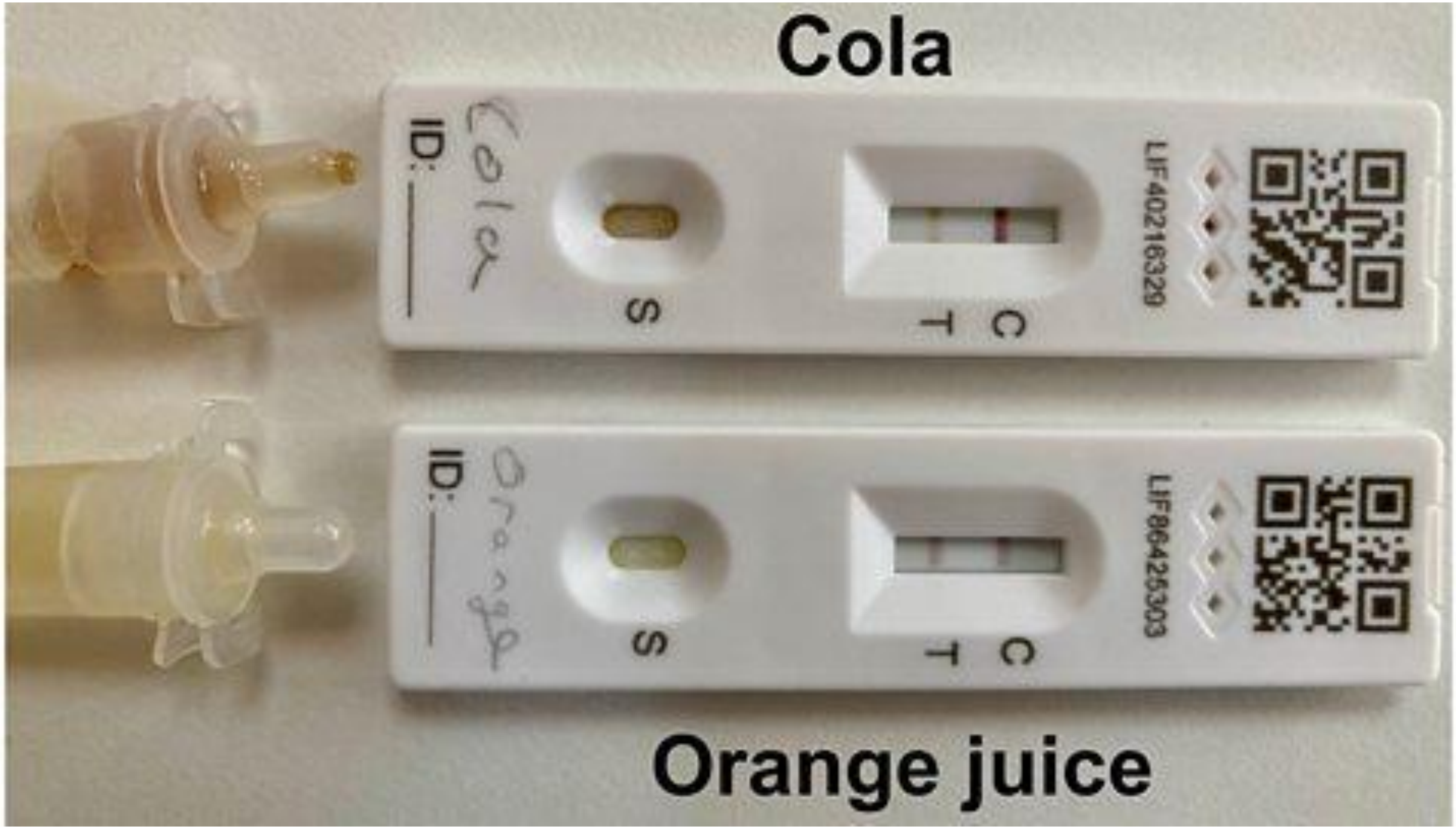
What if we looked deeper?

Trying to find them all – without cherry-picking

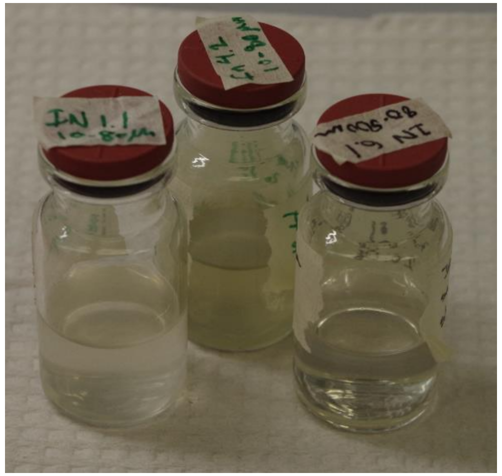
Sometimes you overlock particles when analyzing – false negatives



You cannot blindly trust your analytics – false positives



The journey from matrix to something your instrument can analyze



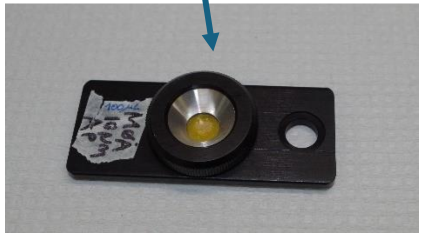
IR or Raman spectroscopy

To get from concentrate to IR-spectra

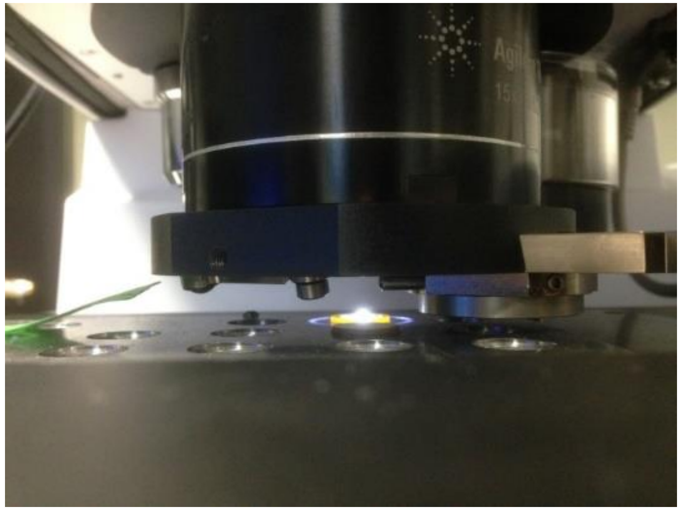
Sample pre-treatment

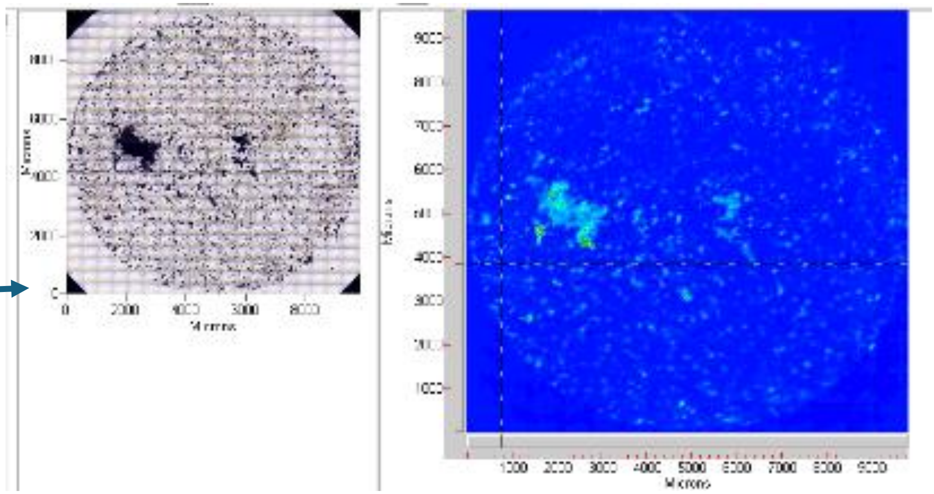
Collect samples in vial

Deposit sample on slide, window or filter

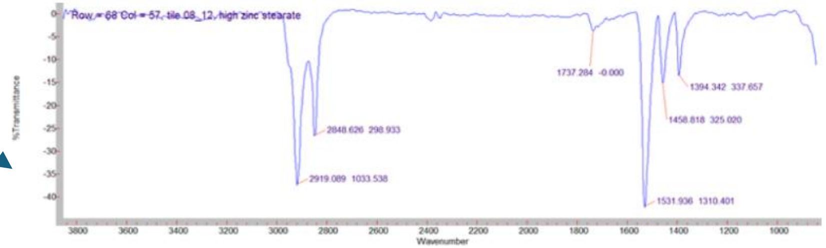


Scan it

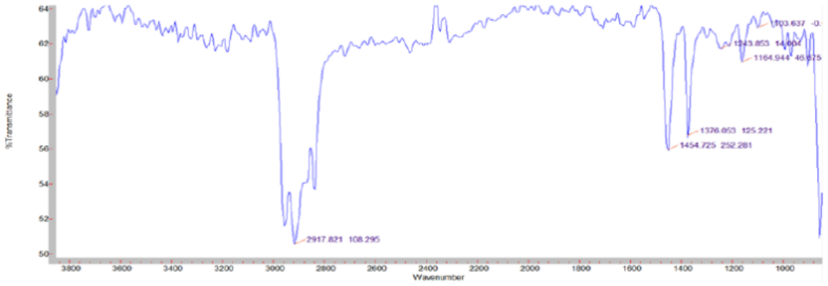




Interpret



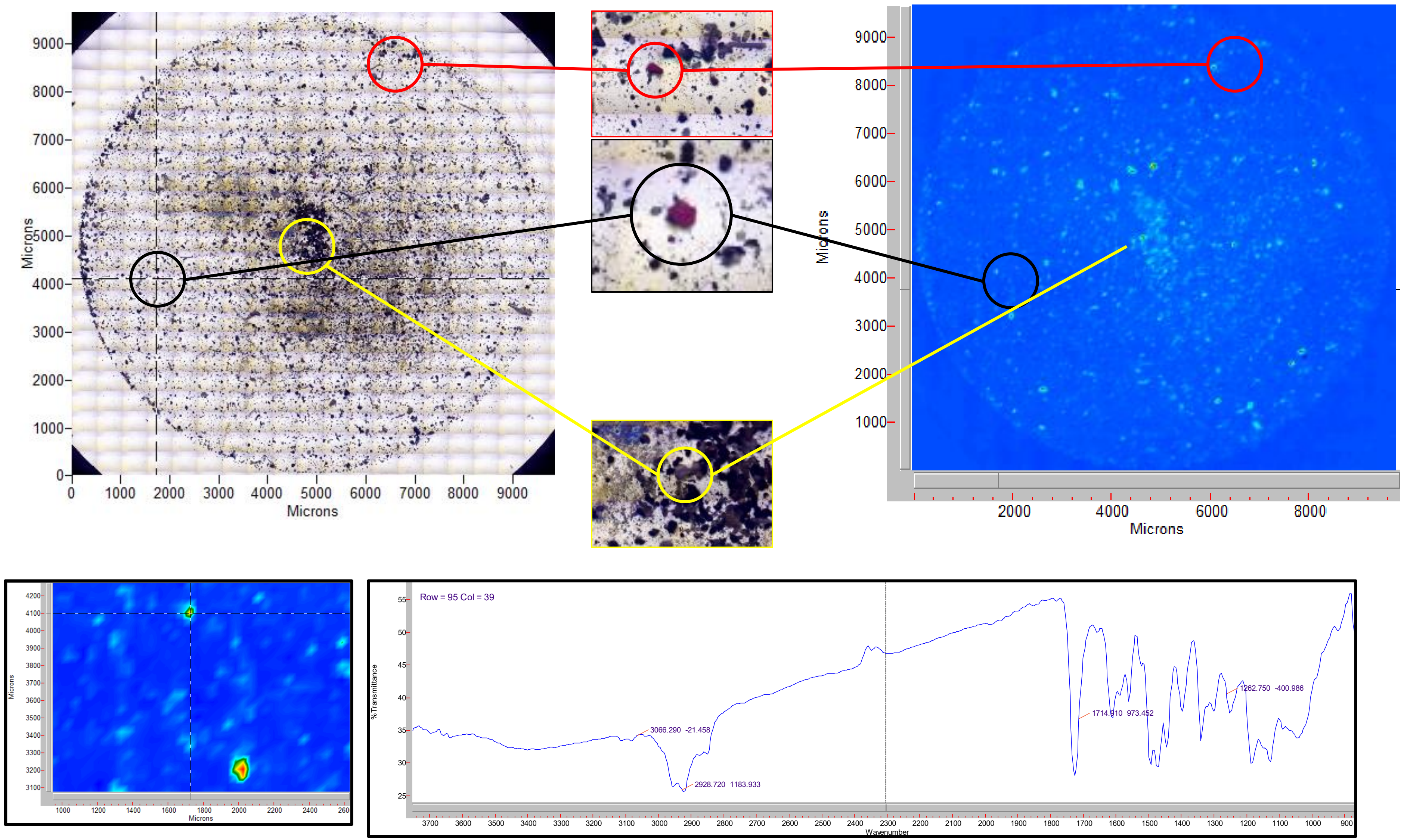
A good IR spectrum of what looks like zinc stearate



A medium quality spectrum of what likely is polypropylene

And out comes the data

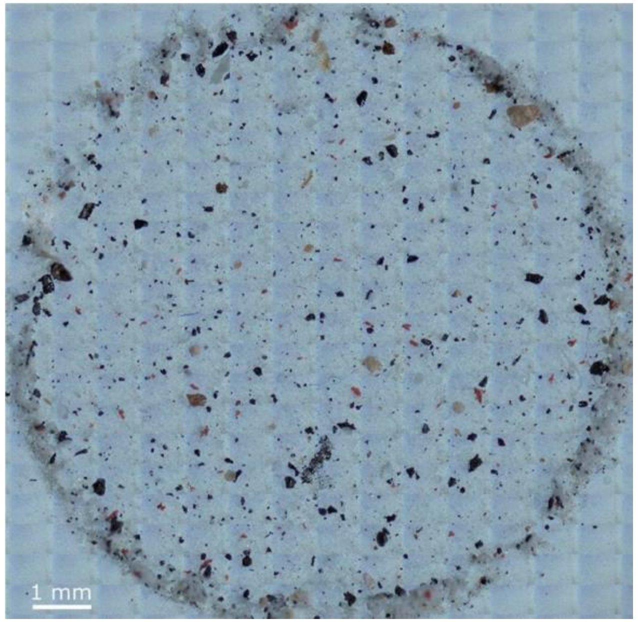
In the beginning we ‘clicked’ each particle

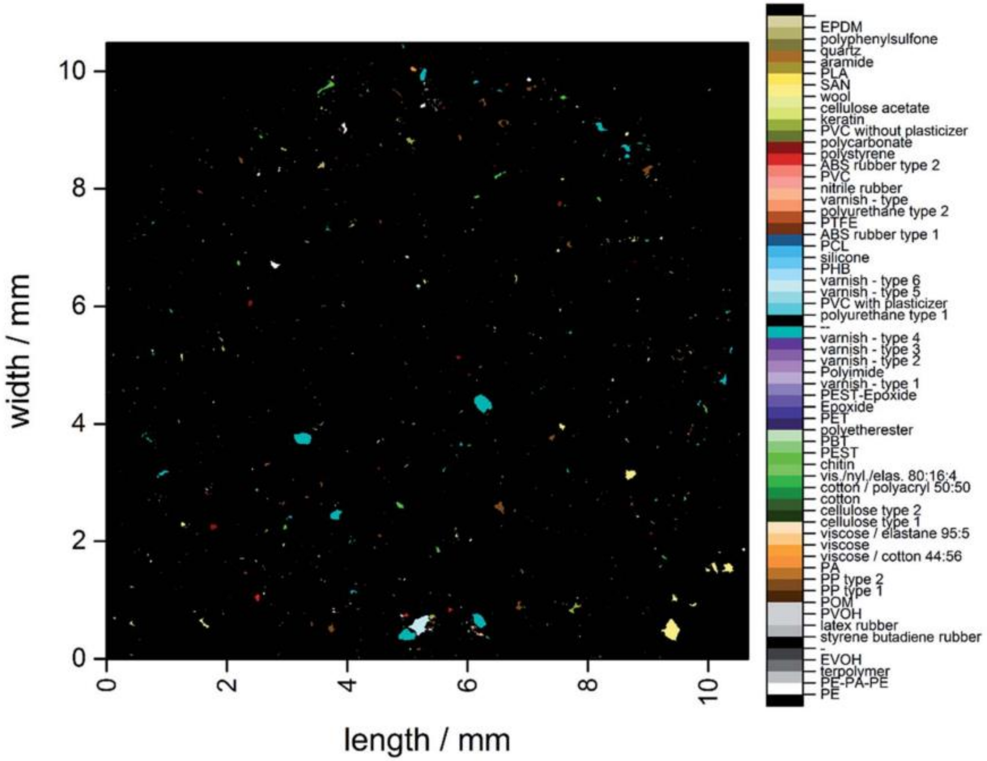


But we got very tired of that

Only part of the window could be analyzed
(one whole window would take a month of work)
Human bias was far too large

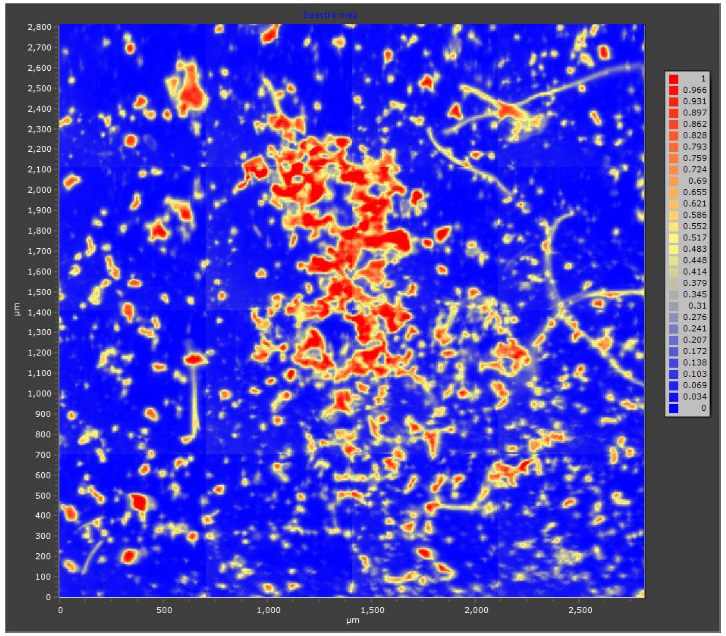
Along came the first automated approach:
Primpke et al., 2017, from Alfred Wegener Institute in Germany





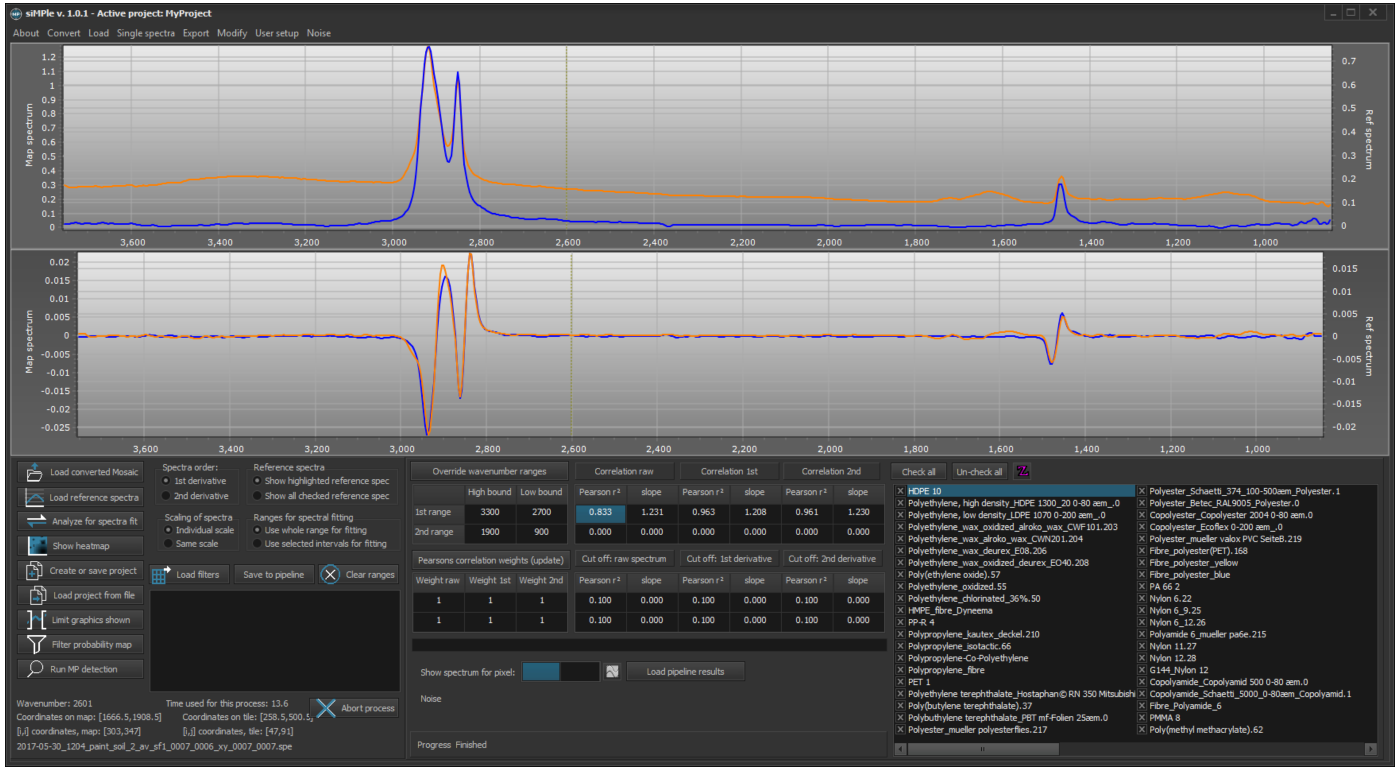
First we build our own software, then integrated with the AWI approach into: siMPle

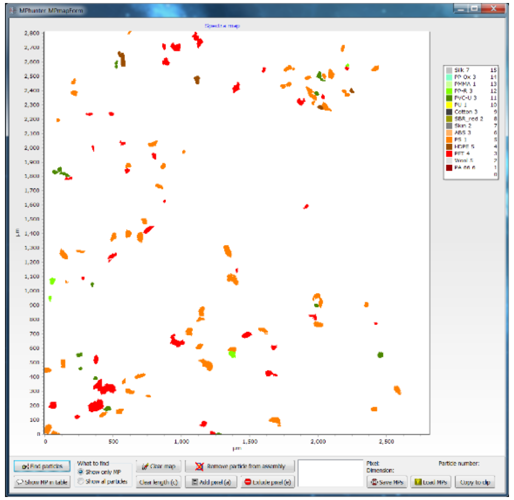
(MP analysis for non-nerds?)

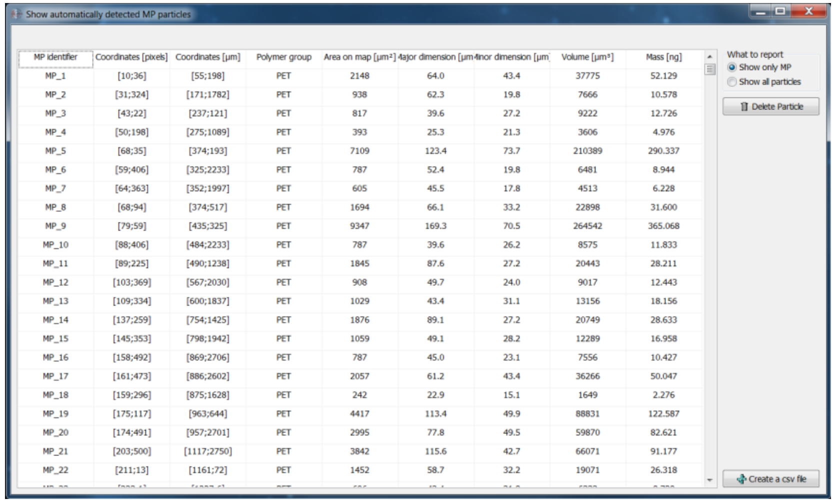


The art of data crunching

We typically scan an area of 10x10 mm at 5.5 µm pixel resolution to create a map = 3,211,264 individual spectra







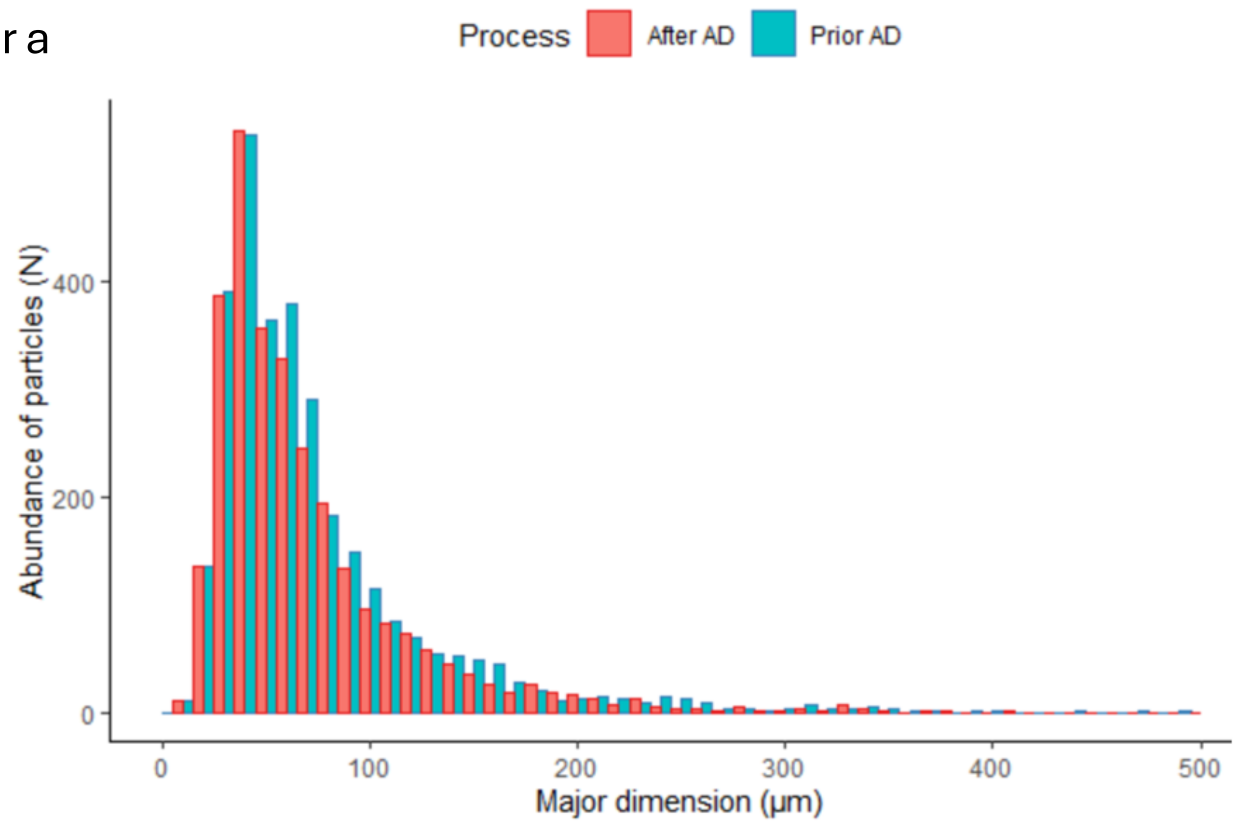
MP identifier	Coordinates [pixels]	Coordinates [µm]	Polymer group	Area on map [µm²]	Major dimension [µm	Minor dimension [µm]	Volume [µm³]	Mass [ng]
MP_1	[10;36]	[55;198]	PET	2148	64.0	43.4	37775	52.129
MP_2	[31;324]	[171;1782]	PET	938	62.3	19.8	7666	10.578
MP_3	[43;22]	[237;121]	PET	817	39.6	27.2	9222	12.726
MP_4	[50;198]	[275;1089]	PET	393	25.3	21.3	3606	4.976
MP_5	[68;35]	[374;193]	PET	7109	123.4	73.7	210389	290.337
MP_6	[59;406]	[325;2233]	PET	787	52.4	19.8	6481	8.944
MP_7	[64;363]	[352;1997]	PET	605	45.5	17.8	4513	6.228
MP_8	[68;94]	[374;517]	PET	1694	66.1	33.2	22898	31.600
MP_9	[79;59]	[435;325]	PET	9347	169.3	70.5	264542	365.068
MP_10	[88;406]	[484;2233]	PET	787	39.6	26.2	8575	11.833
MP_11	[89;225]	[490;1238]	PET	1845	87.6	27.2	20443	28.211
MP_12	[103;369]	[567;2030]	PET	908	49.7	24.0	9017	12.443
MP_13	[109;334]	[600;1837]	PET	1029	43.4	31.1	13156	18.156
MP_14	[137;259]	[754;1425]	PET	1876	89.1	27.2	20749	28.633
MP_15	[145;353]	[798;1942]	PET	1059	49.1	28.2	12289	16.958
MP_16	[158;492]	[869;2706]	PET	787	45.0	23.1	7556	10.427
MP_17	[161;473]	[886;2602]	PET	2057	61.2	43.4	36266	50.047
MP_18	[159;296]	[875;1628]	PET	242	22.9	15.1	1649	2.276
MP_19	[175;117]	[963;644]	PET	4417	113.4	49.9	88831	122.587
MP_20	[174;491]	[957;2701]	PET	2995	77.8	49.5	59870	82.621
MP_21	[203;500]	[1117;2750]	PET	3842	115.6	42.7	66071	91.177
MP_22	[211;13]	[1161;72]	PET	1452	58.7	32.2	19071	26.318

www.simple-plastics.eu/

µFTIR imaging with automated analysis finds more microplastics

But it does not find them all !!!

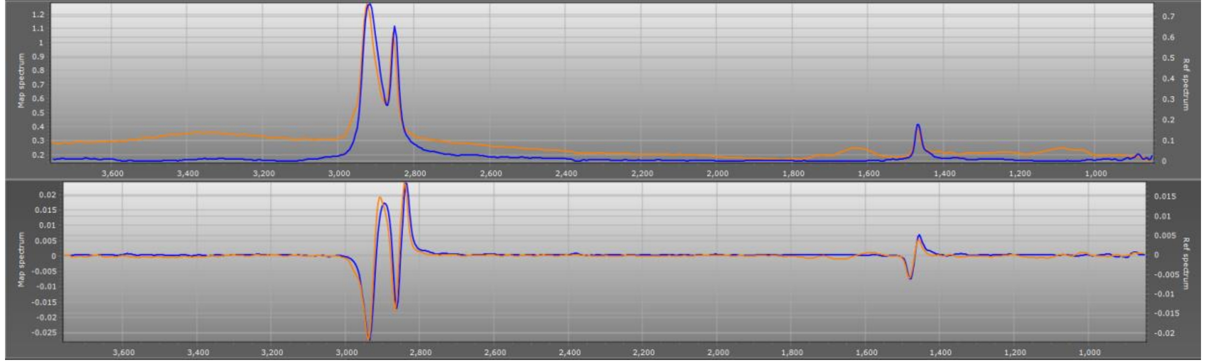
Size of microplastics before and after a mesophilic anaerobic digestion



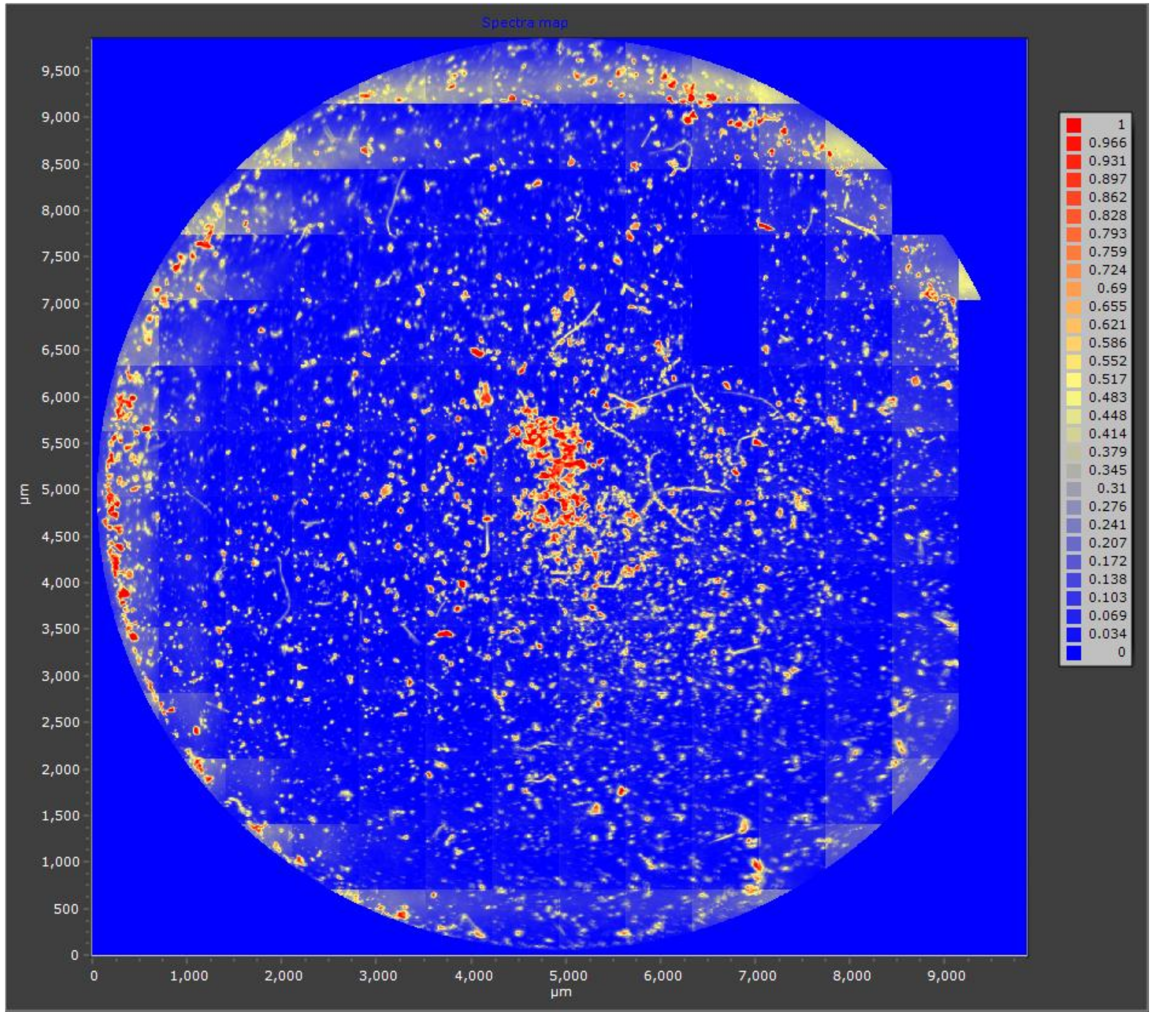
Chand et al. (in prep)

An example, a soil from a harbor

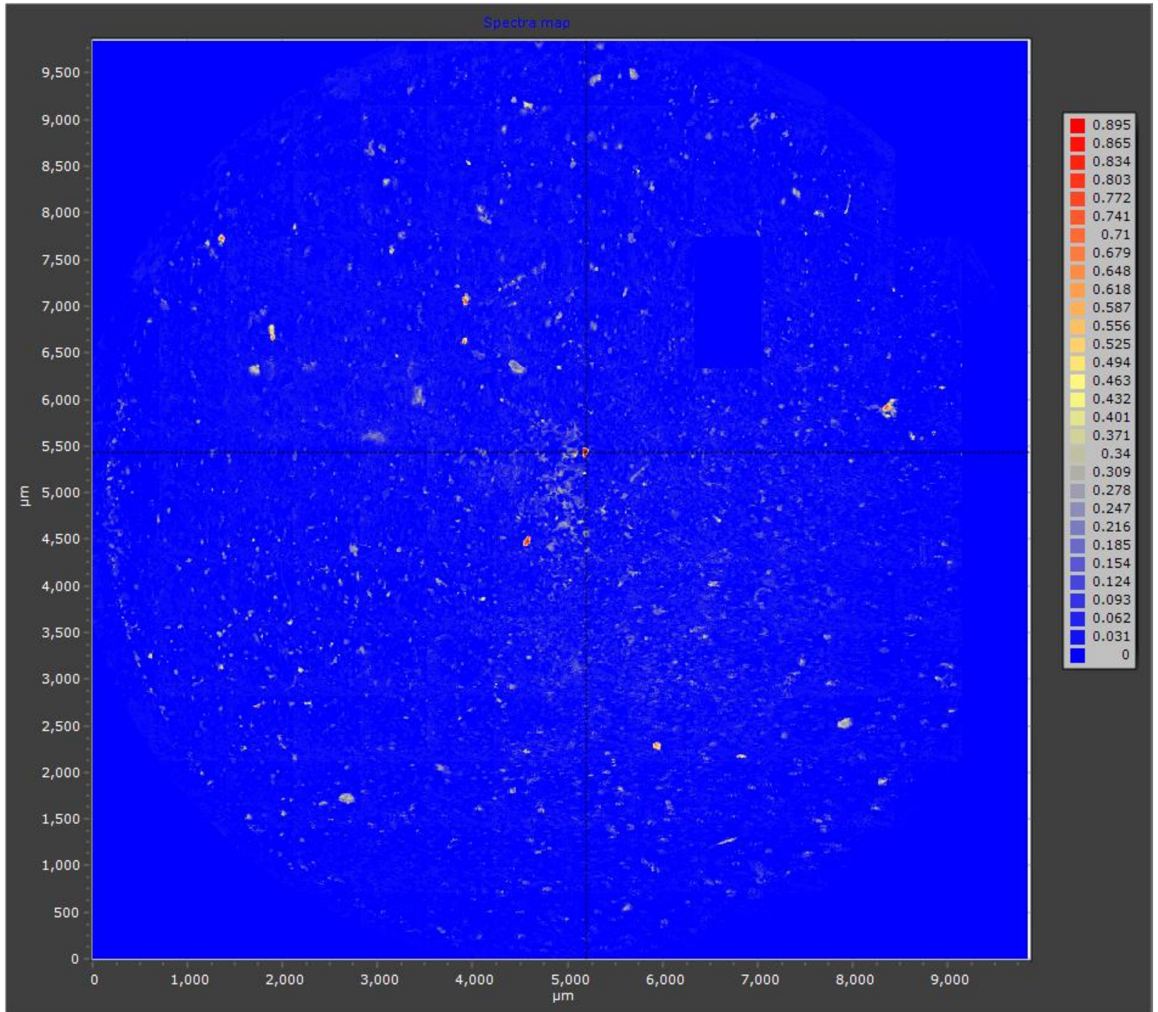
(sorry for the missing tiles)

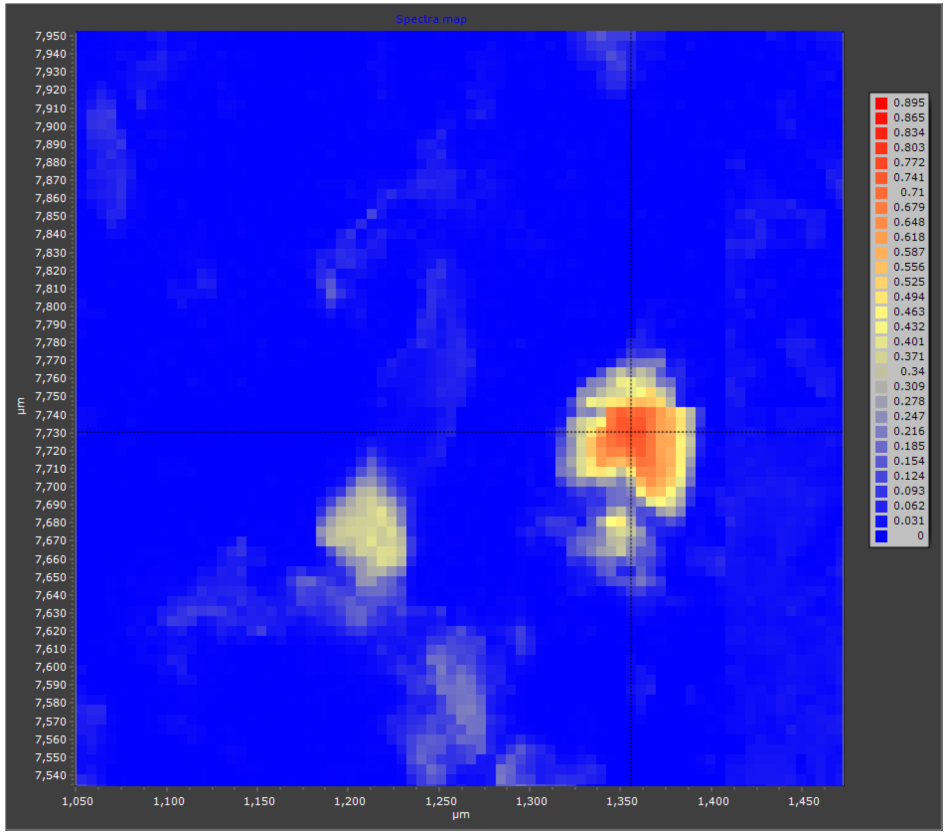


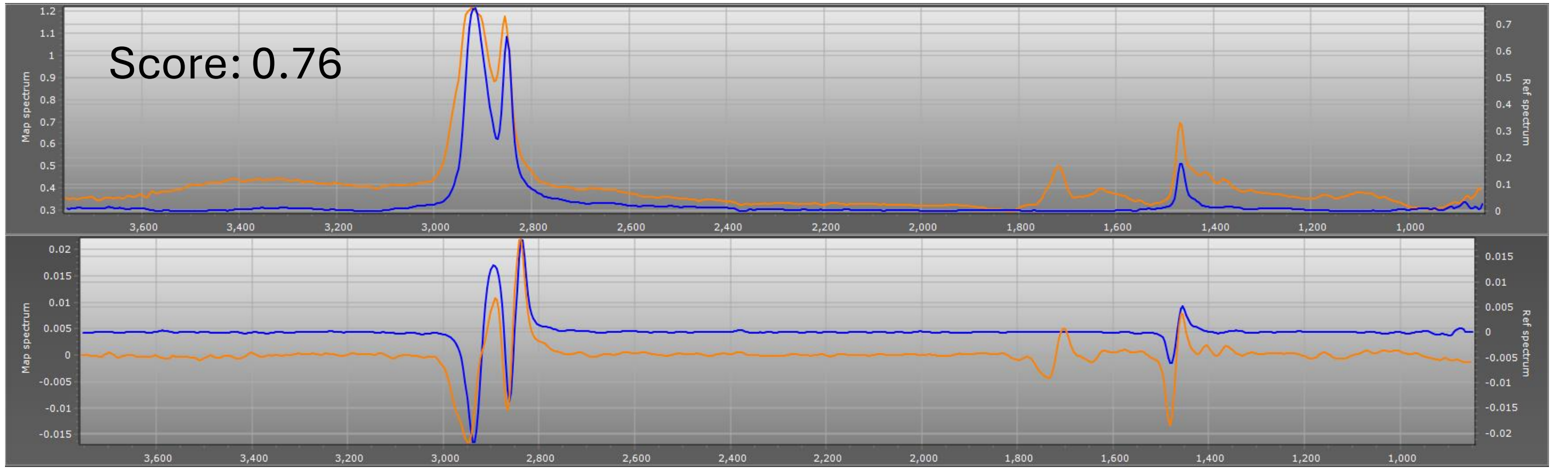
Absorbance at 2000 cm^{-1}



Filtering for correlation to one HDPE spectrum





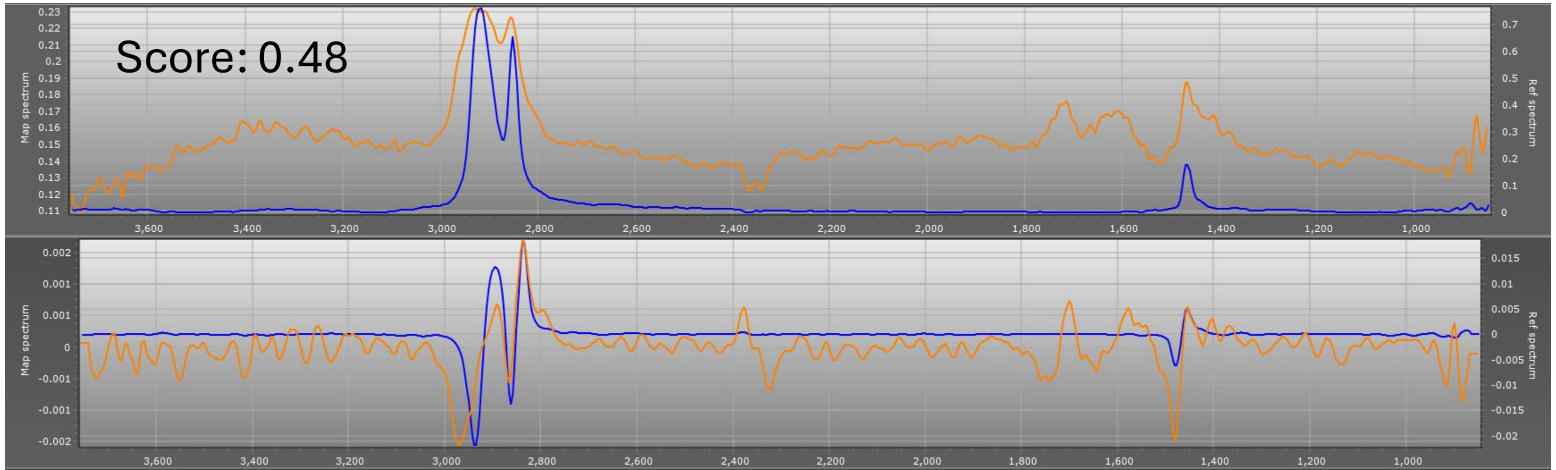


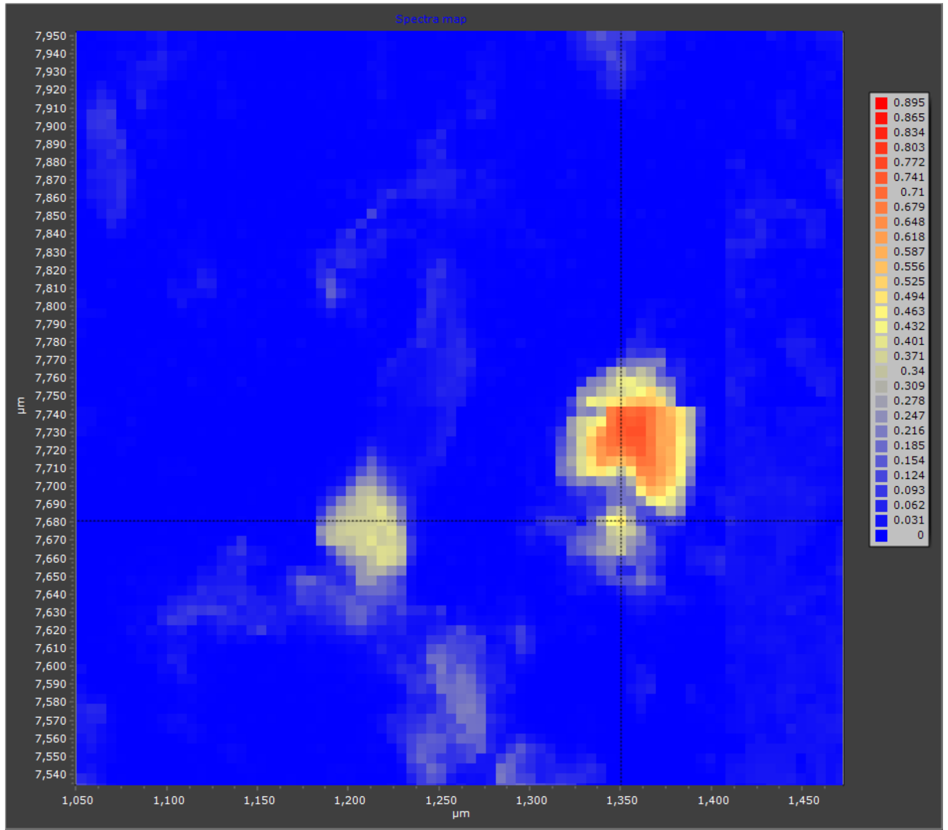
This is a PE particle with a nice fit to raw spectrum and 1st derivate

This gets recognized as MP

This gets overlooked

This is probably a PE particle with a poor fit to raw spectrum and 1st derivate





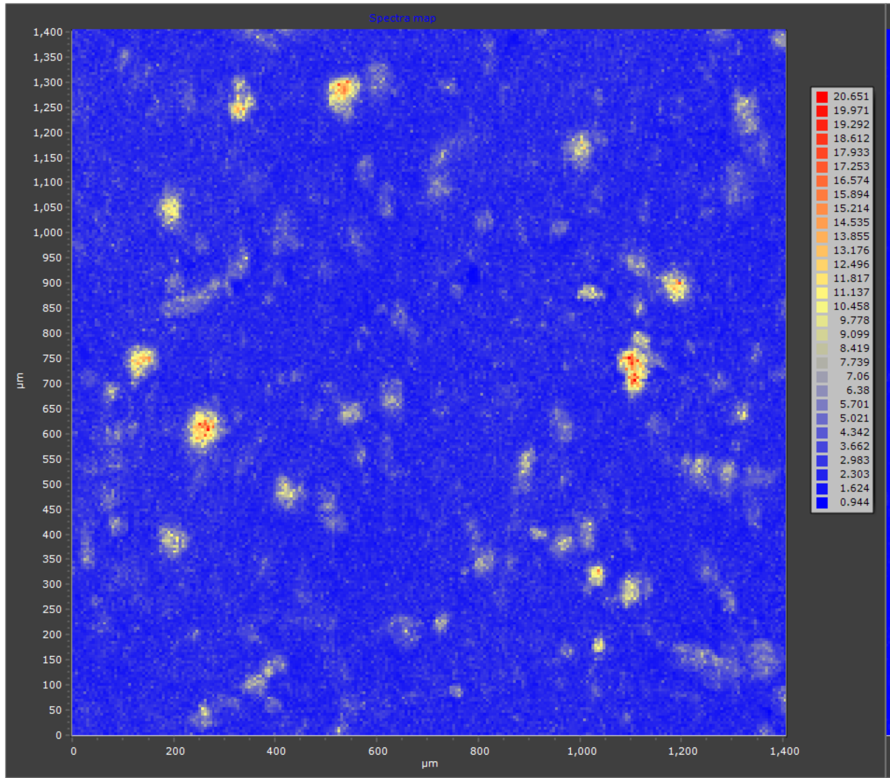
Why do small particles get overlooked even by imaging?

Spectra are deteriorated due to aging of the material (can be considered by the choice of database)

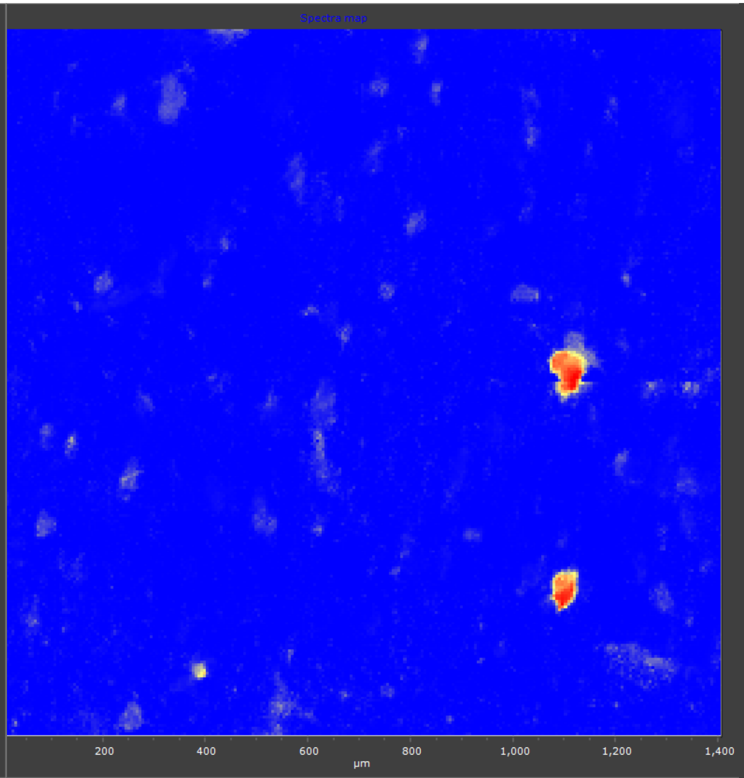
Particles get so thin that the signal (peaks) are over-shadowed by noise (random fluctuations)

Probably we also loose small particles in the sample preparation and microplastics extraction

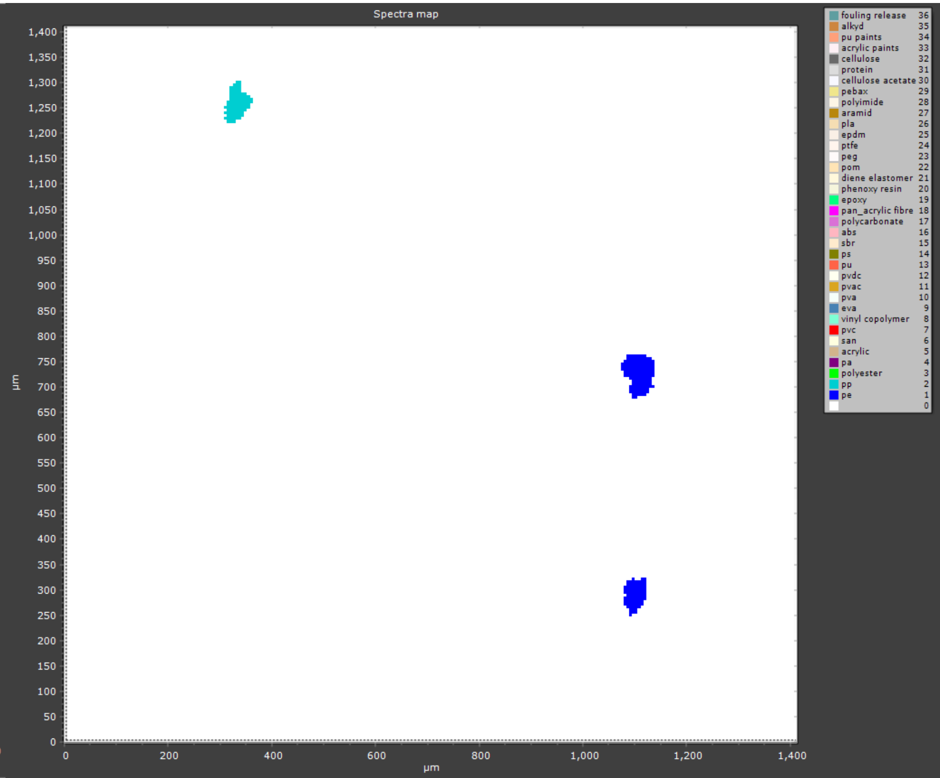
A signal-to-noise analysis



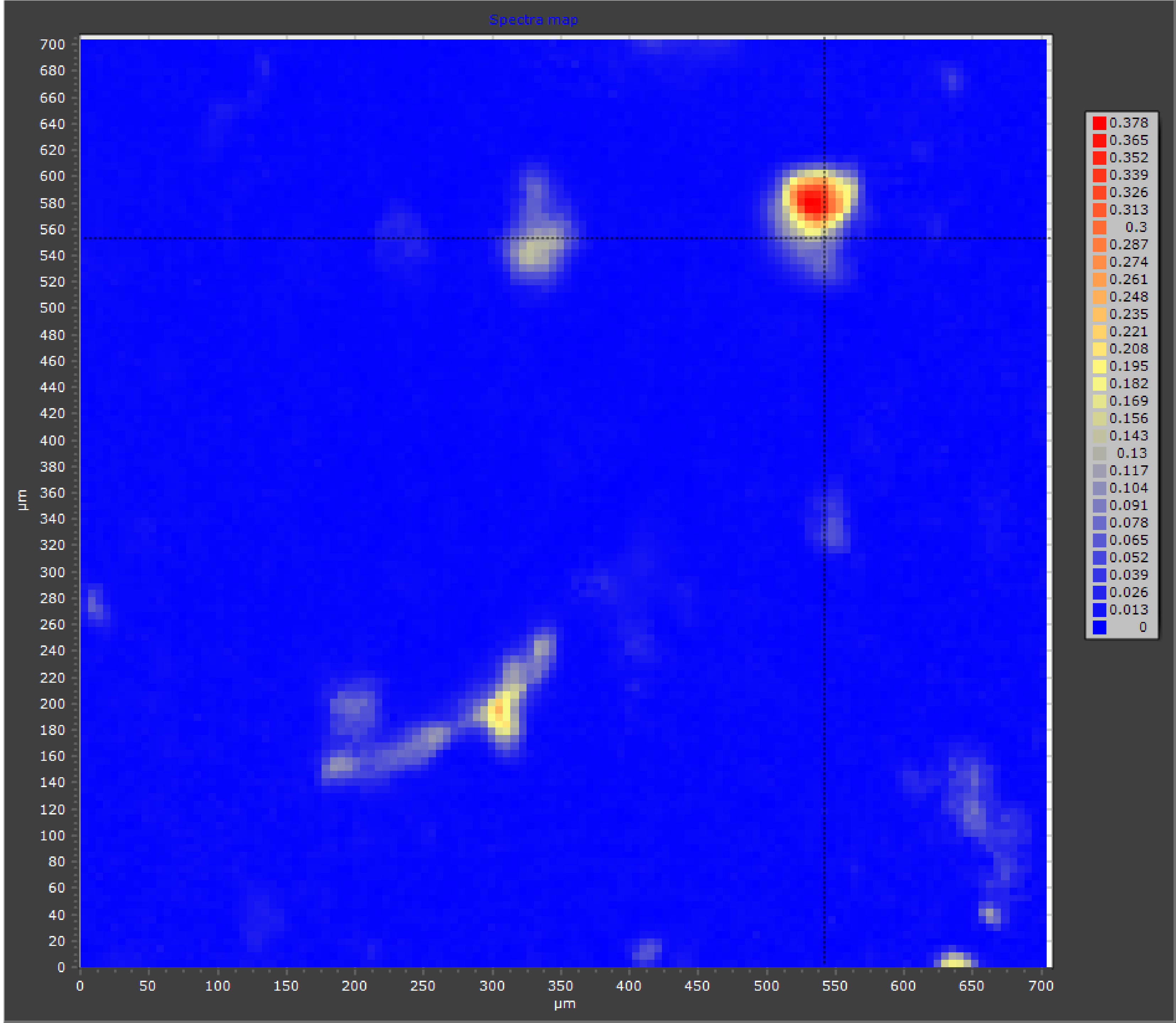
And a correlation to a HDPE spectrum



And detected microplastics



Heatmap – one tile only (0.7 mm)



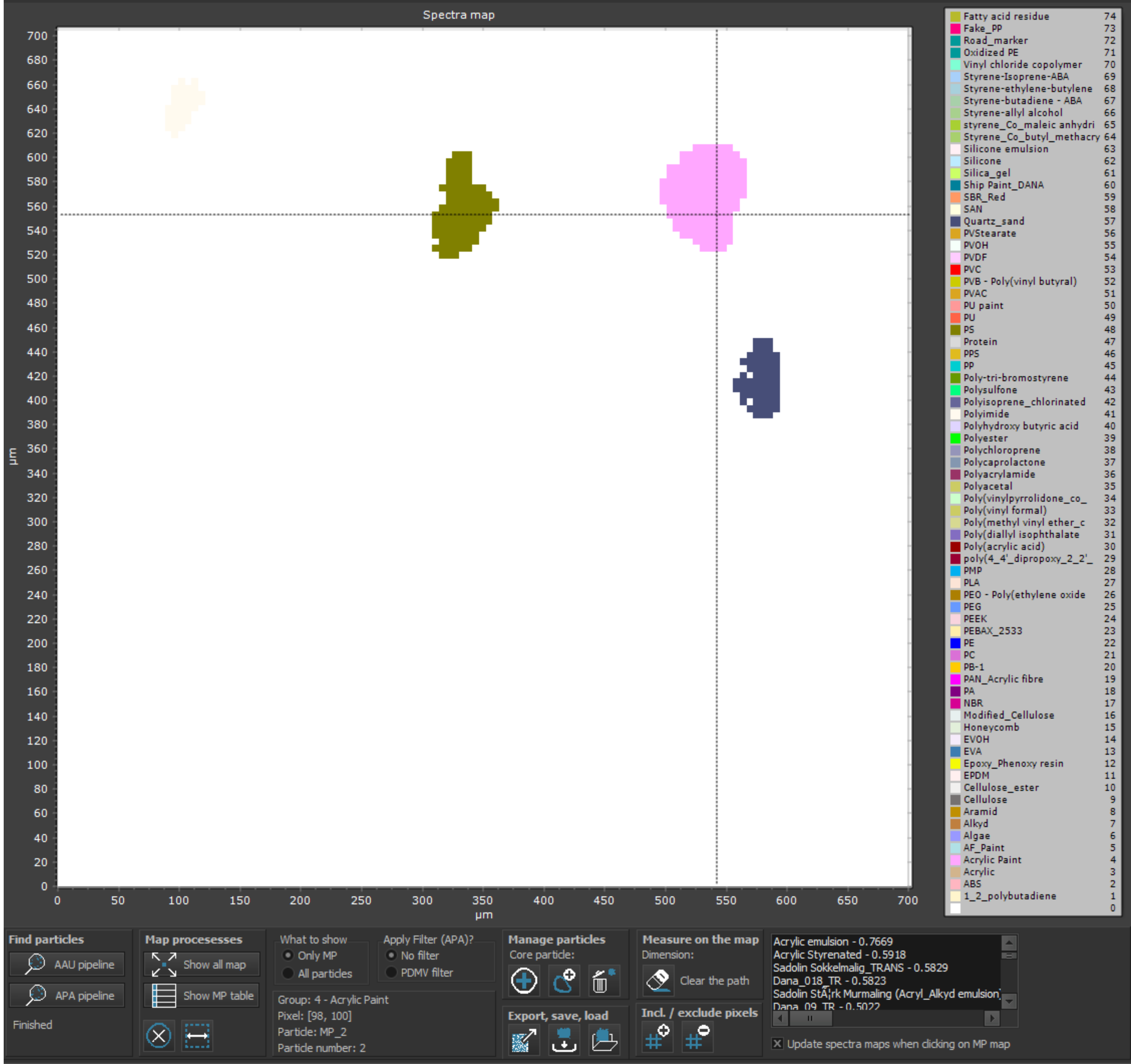
Heatmap shown at 1735 cm^{-1}

Using the AAU pipeline at quite conservative database thresholds

This pipeline does not allow 1-pixel particles

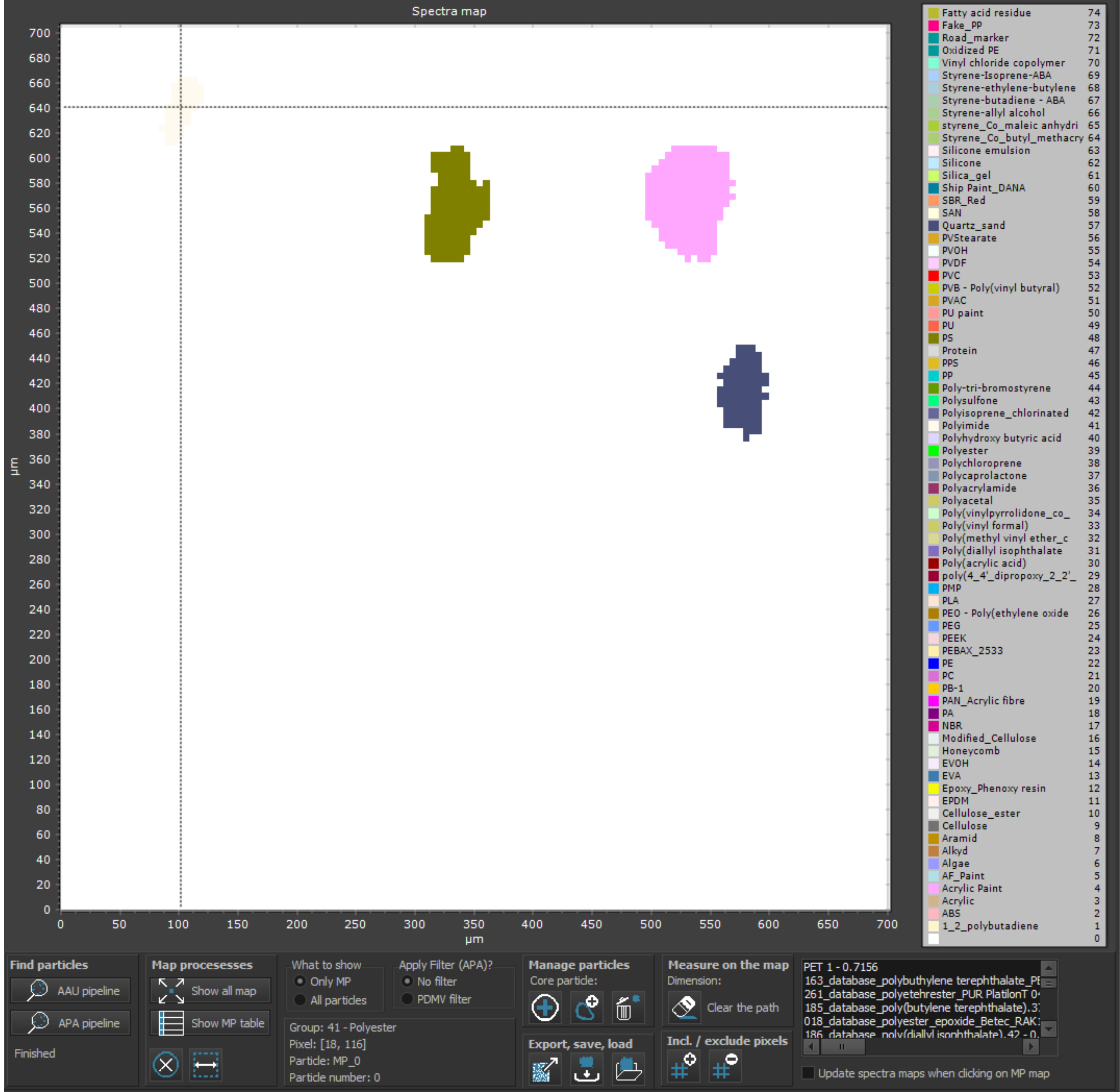
Searching with a paint-focused database

3 particles identified



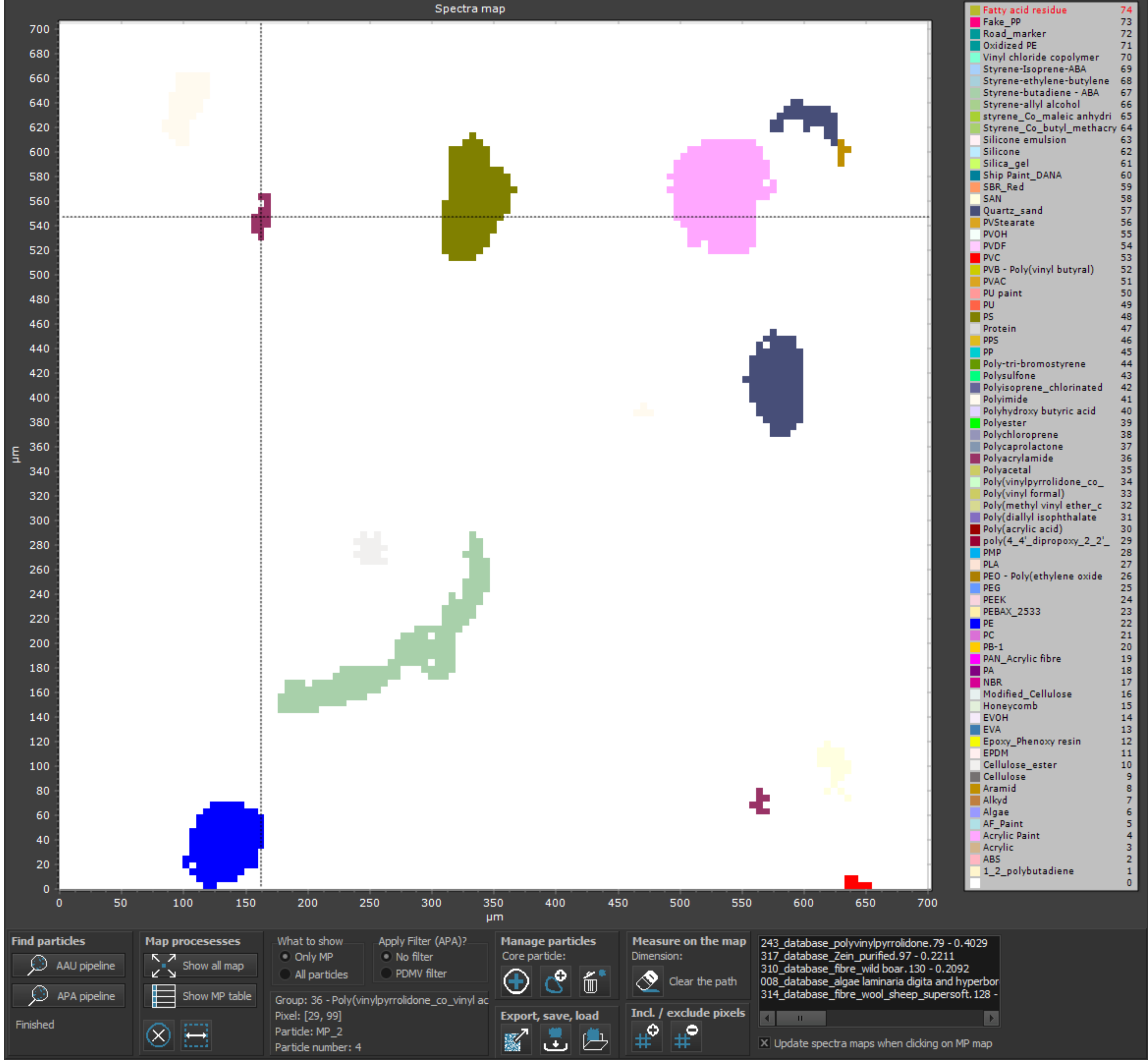
Using the AAU pipeline at slightly more relaxed database thresholds

4 particles identified



Using the AAU pipeline at significantly more relaxed database thresholds

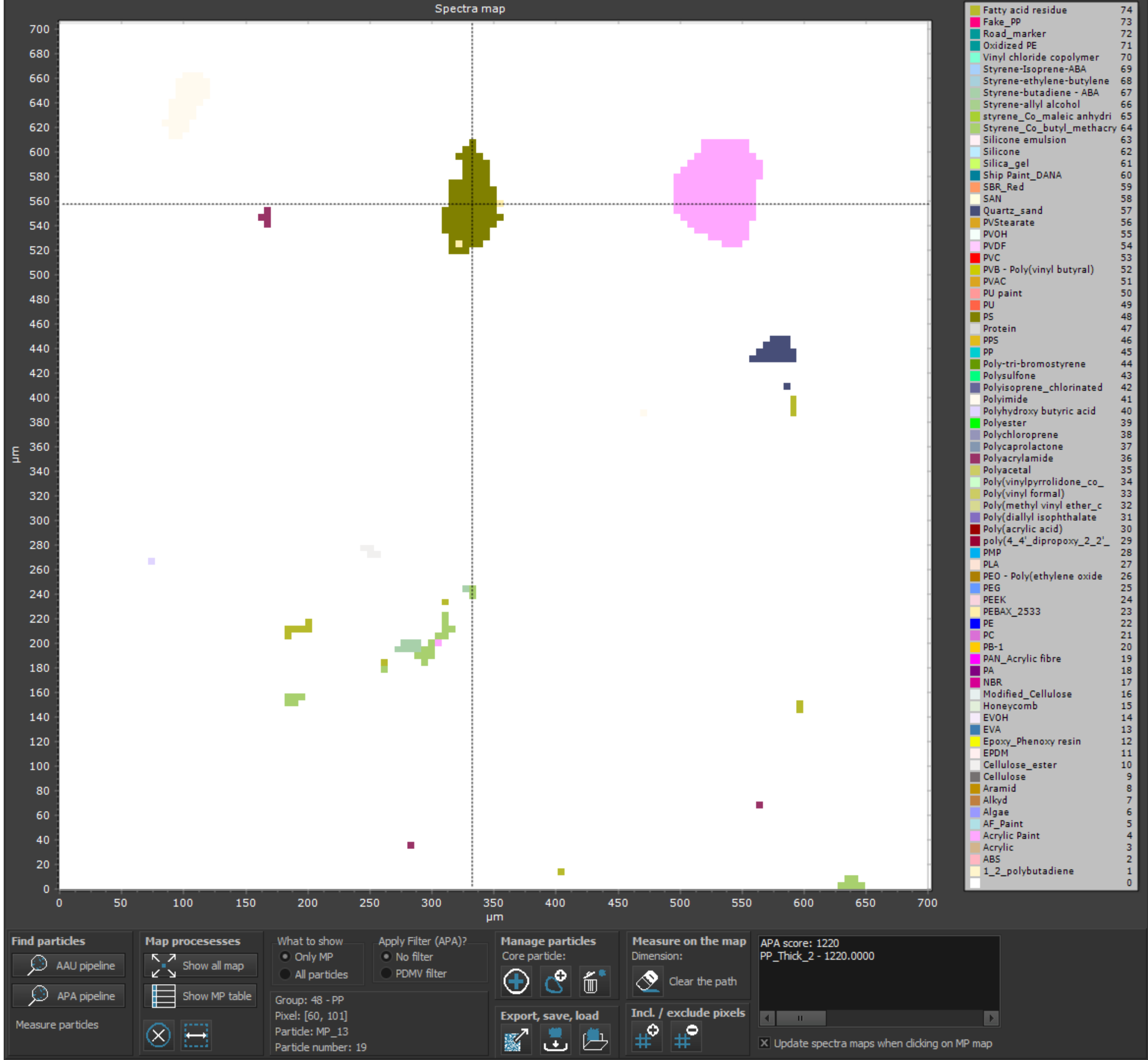
13 particles identified



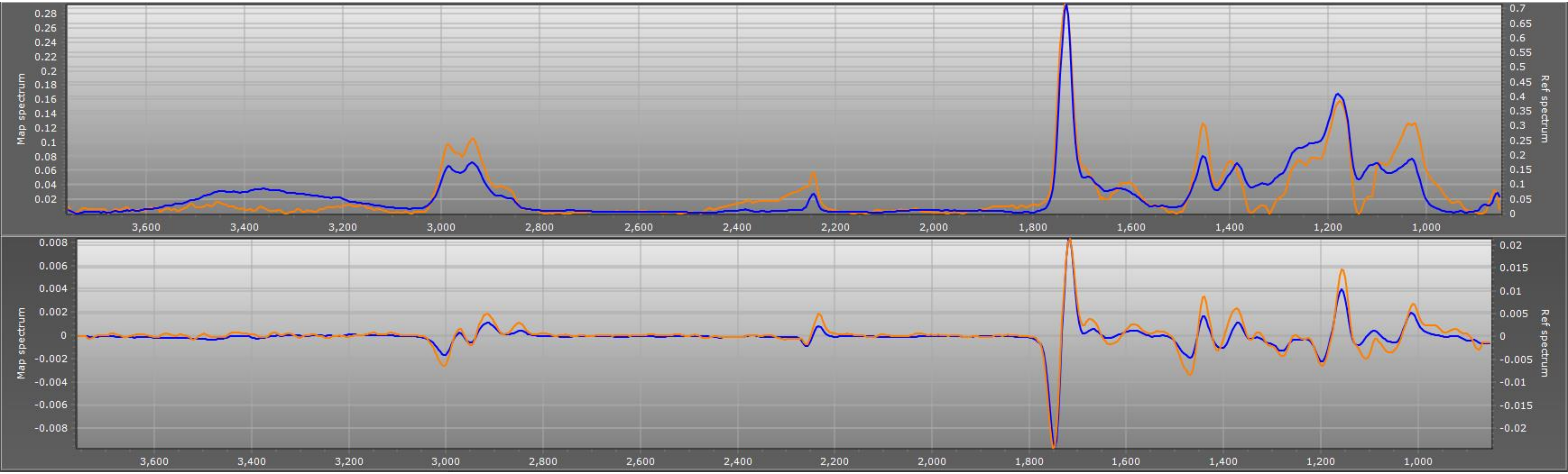
Using the APA pipeline at quite relaxed database thresholds.

This pipeline allows 1-pixel particles

26 particles identified



Finding a balance between false positives and false negatives – when is a match “good enough”



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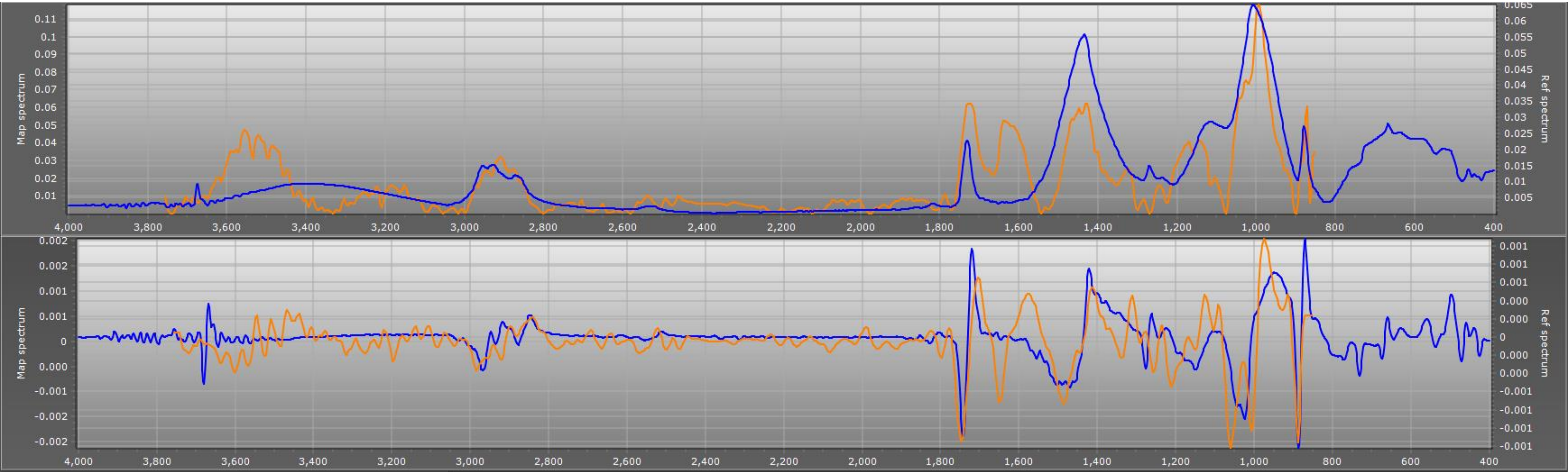

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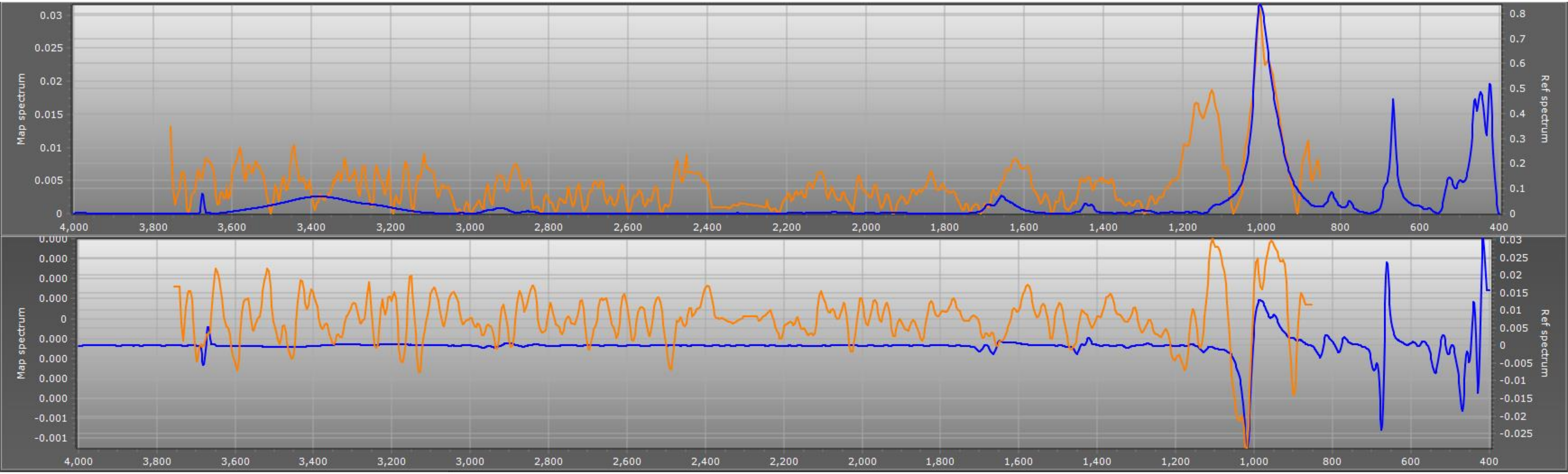


So, Let’s Get Going
(when the going get’s tough, and so on)

Using AI and large-scale spectral databases for polymer identification of microplastics

- a chemometric perspective on the problem of creating data-agnostic software for microplastics analysis

Dr. Benedikt Hufnagl

Hufnagl Chemometrics

Agenda

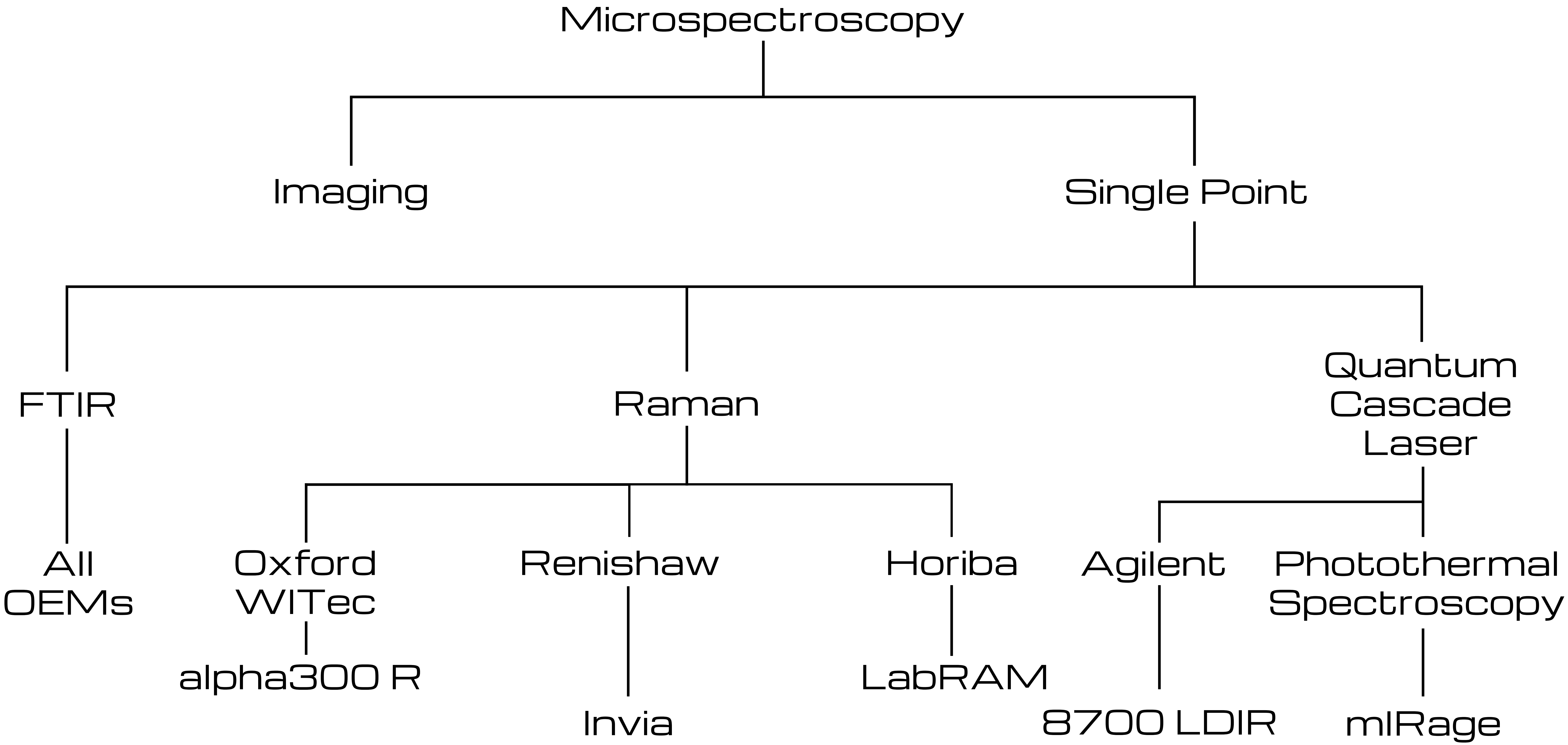
Commonly used devices
microparticlesAI
What is machine learning?
Building data-agnostic approaches
Compare and Validate ML models

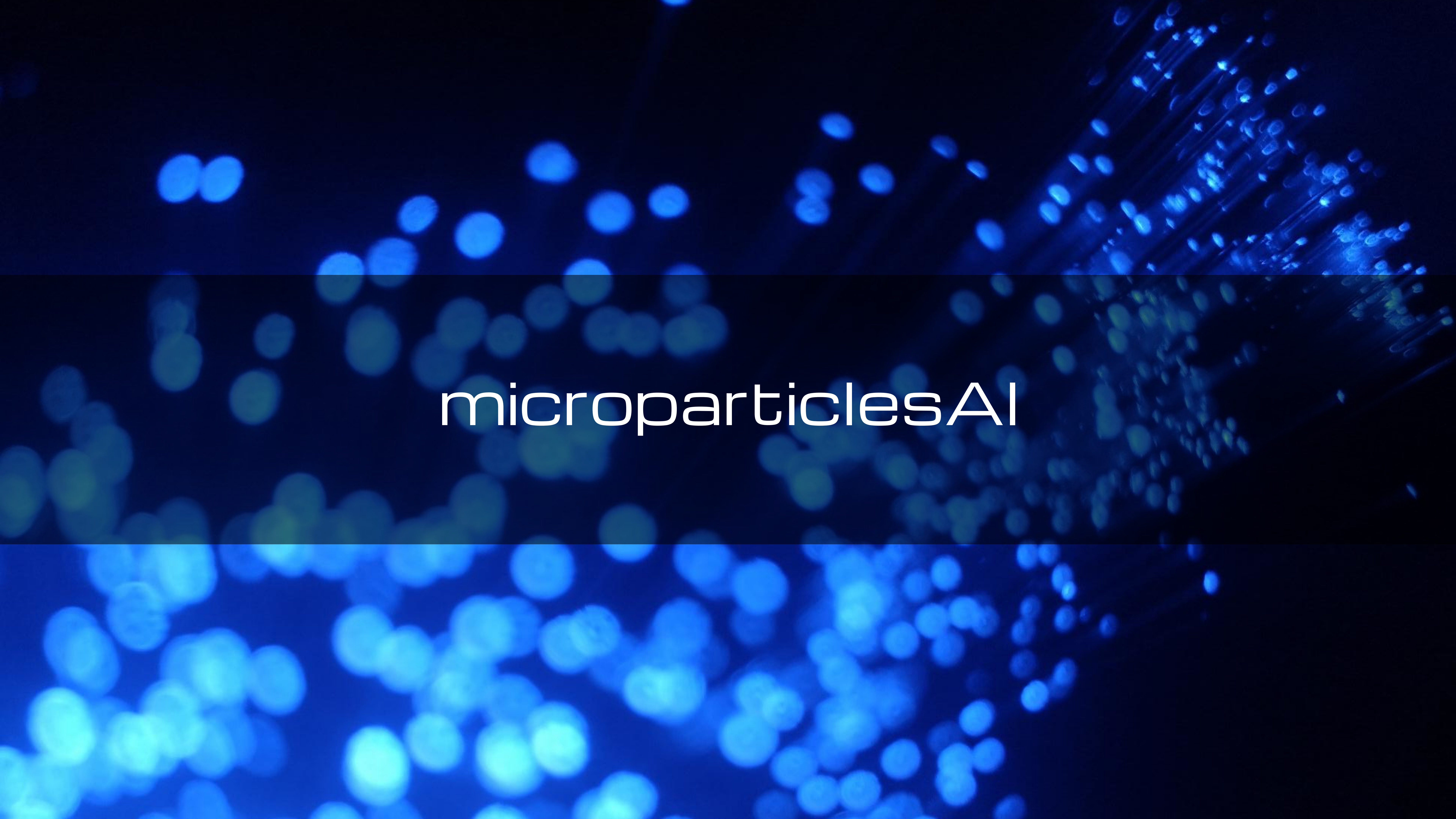
Commonly used devices in microspectroscopy

Commonly used devices for MP analysis

- Microspectroscopy
  - Imaging
    - FTIR (FPA)
      - Bruker
        - Lumos II
        - Hyperion 3000 / II
      - Agilent
        - Cary 620
    - FTIR (Line Array)
      - PerkinElmer
        - Spotlight 400
      - Thermofisher Scientific
        - Nicolet iN10 MX
    - Quantum Cascade Laser
      - DRS Daylight Solutions
        - Spero QT
  - Single Point

Commonly used devices for MP analysis

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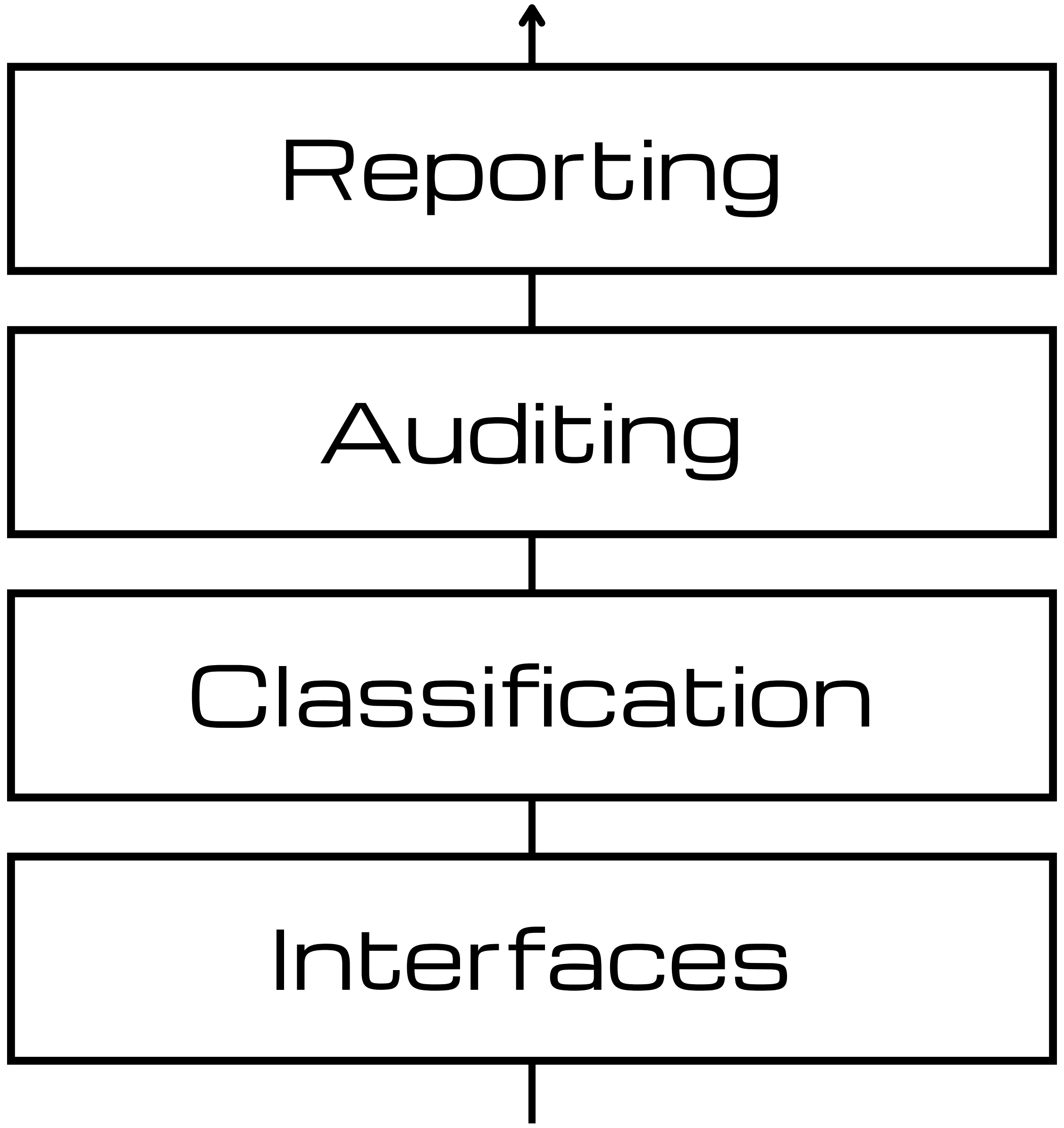
A complex development project



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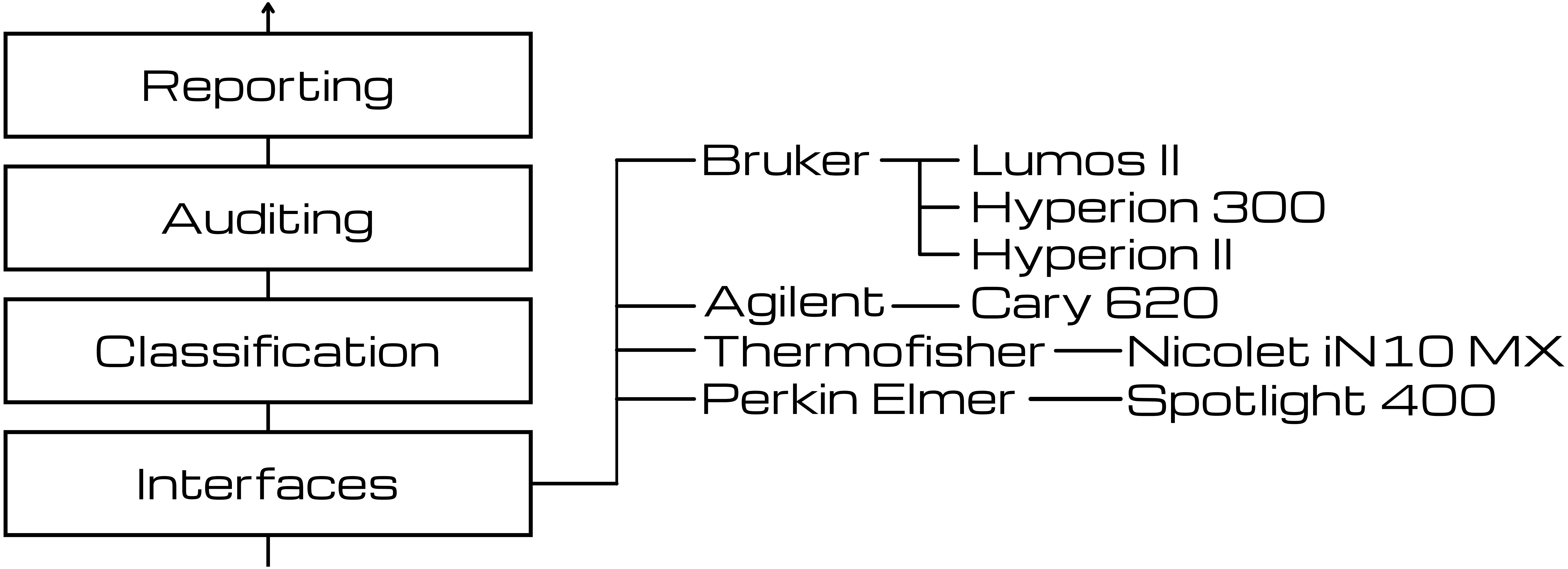

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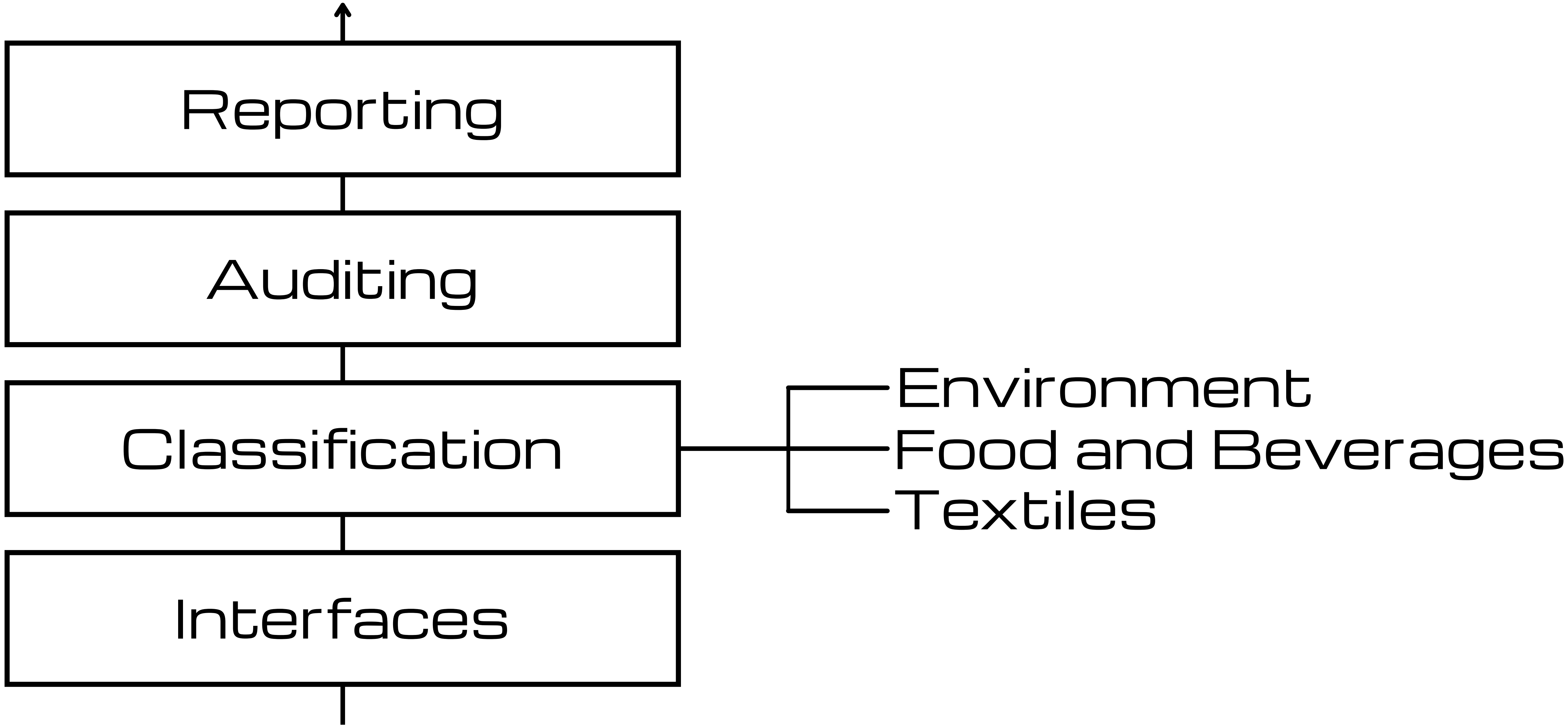

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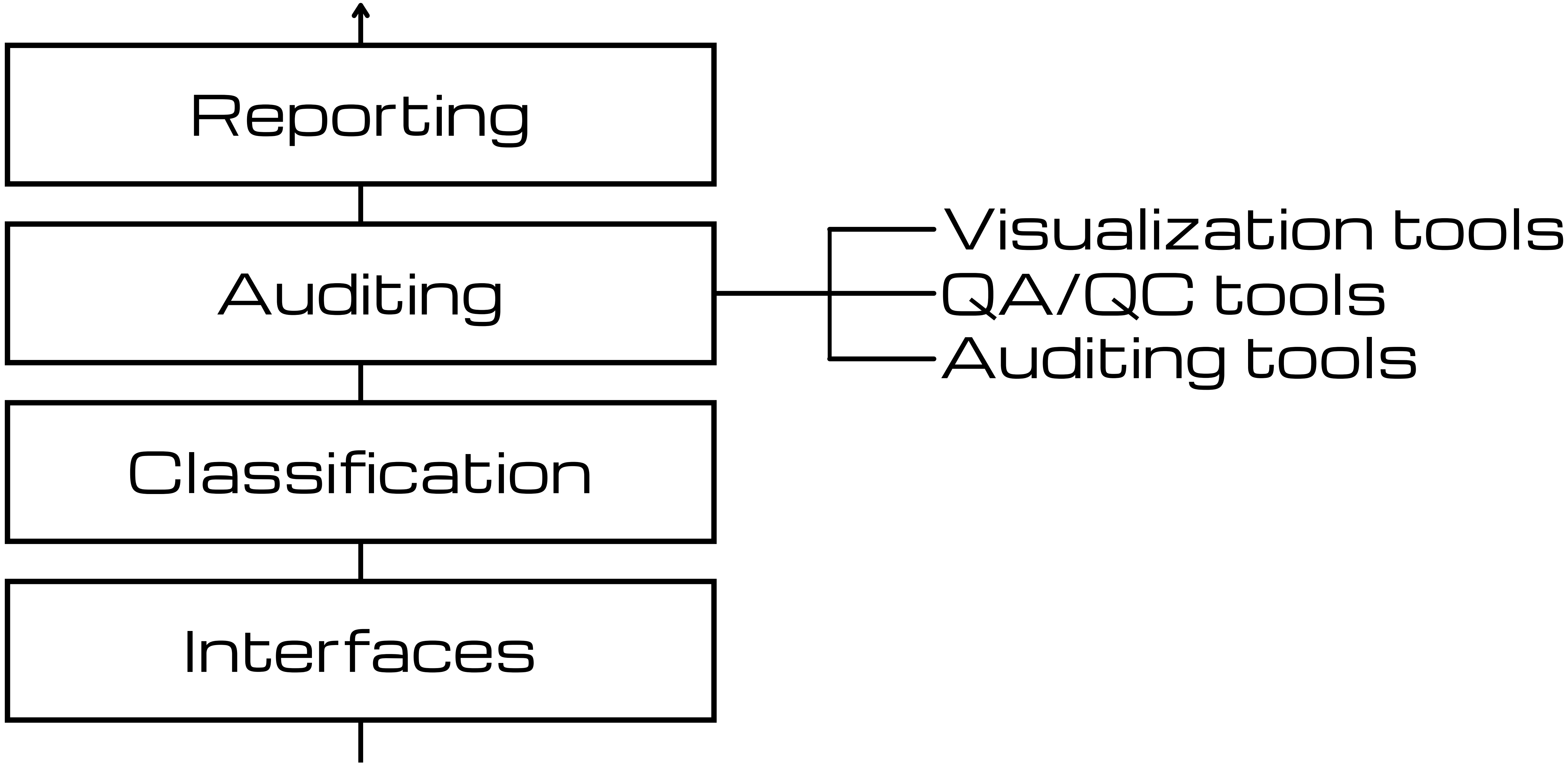

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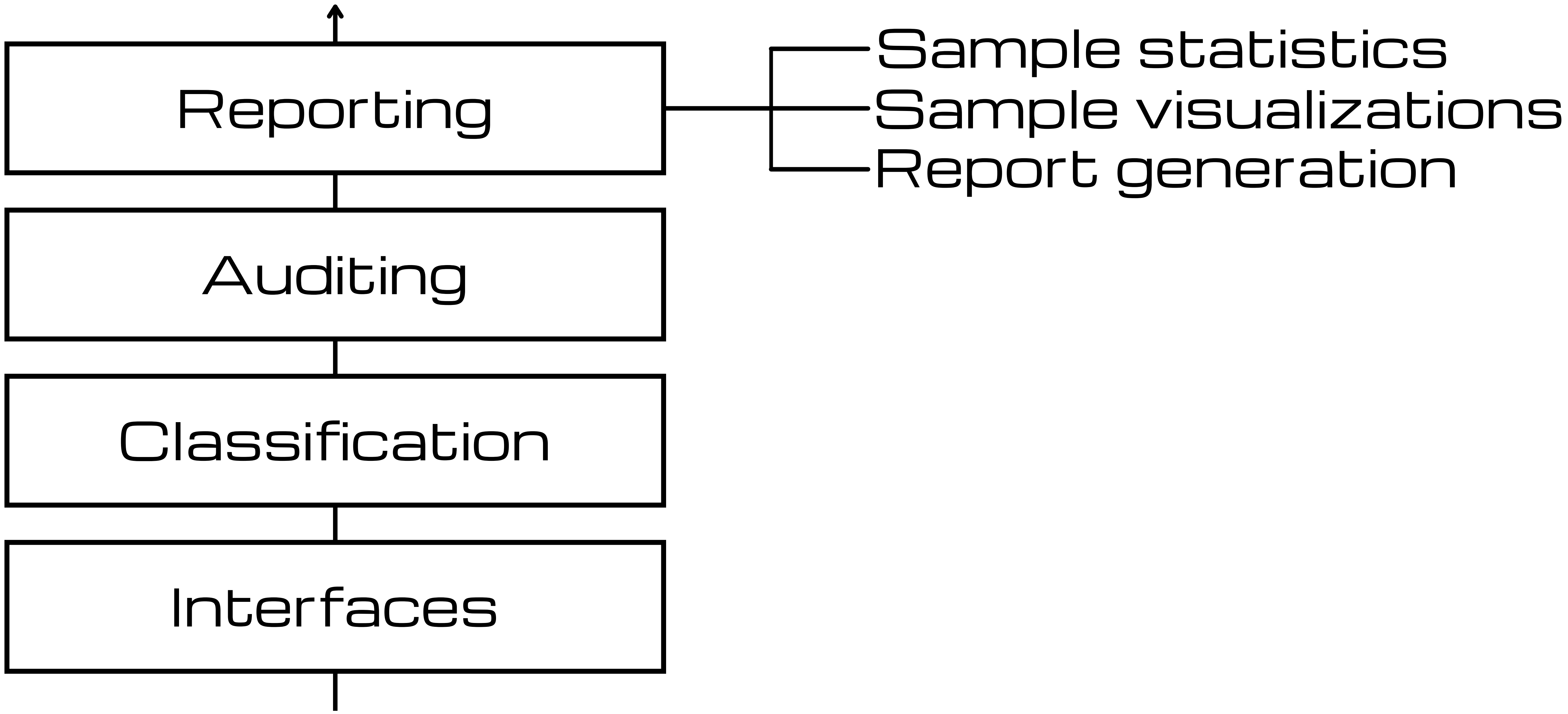

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Multiple devices

One machine learning model

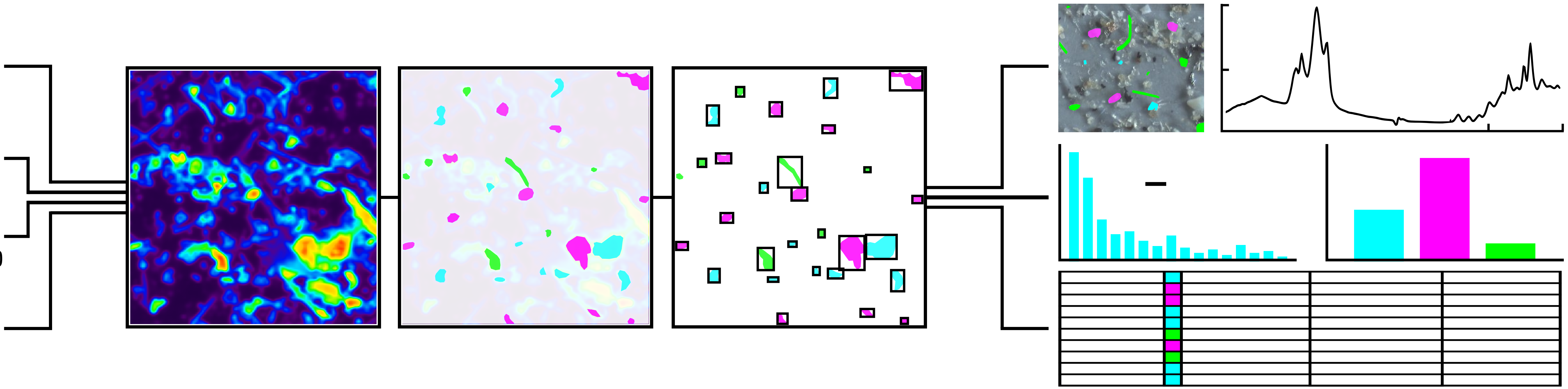
Harmonized result

PerkinElmer
Spotlight 400

Thermofisher
Nicolet iN10 MX

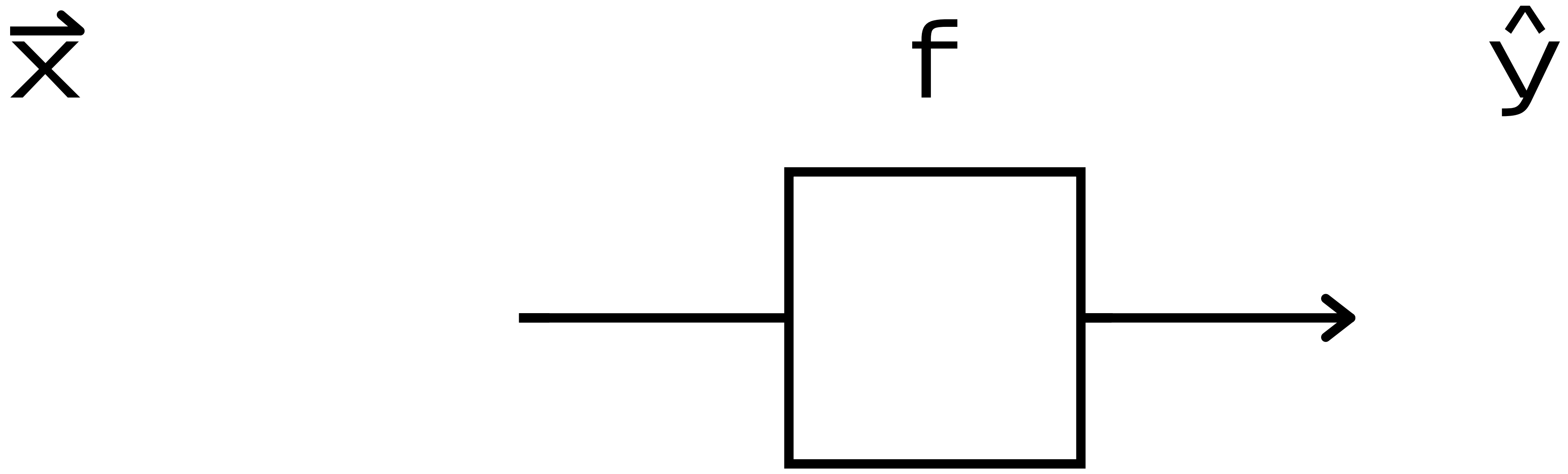
Bruker
Lumos II, Hyperion 3000

Agilent
Cary 620



What is machine learning?

What is a classifier?



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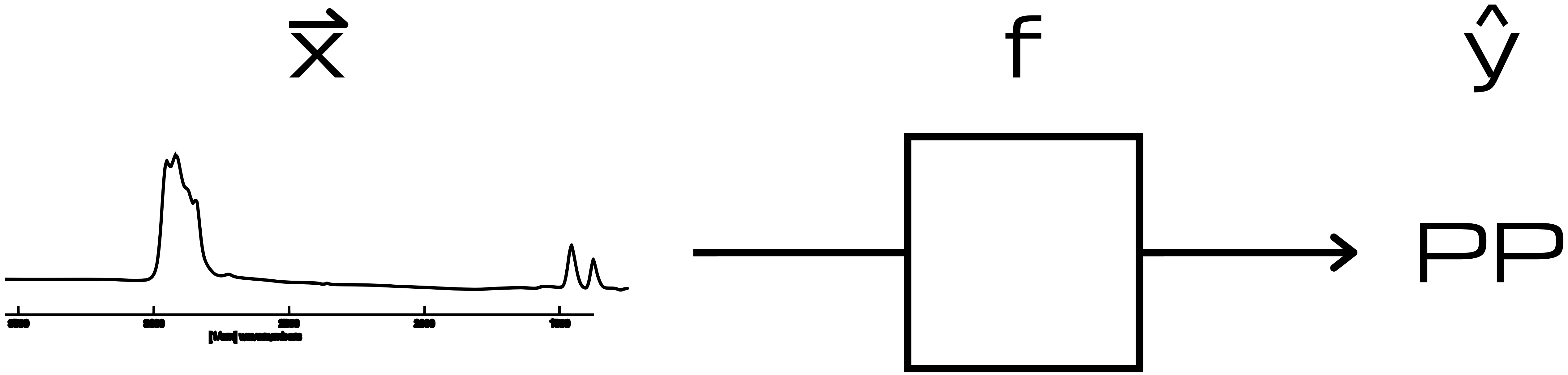

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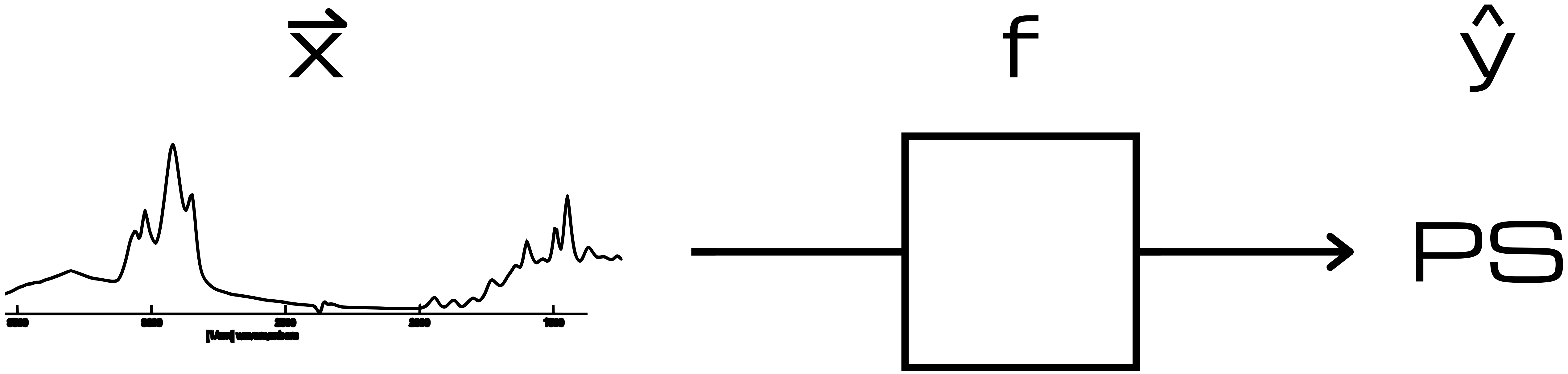

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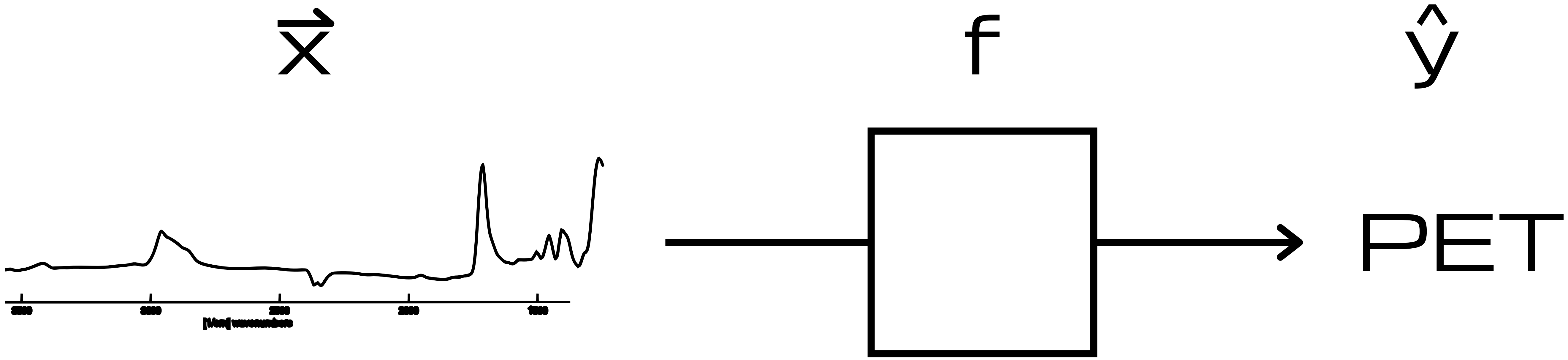
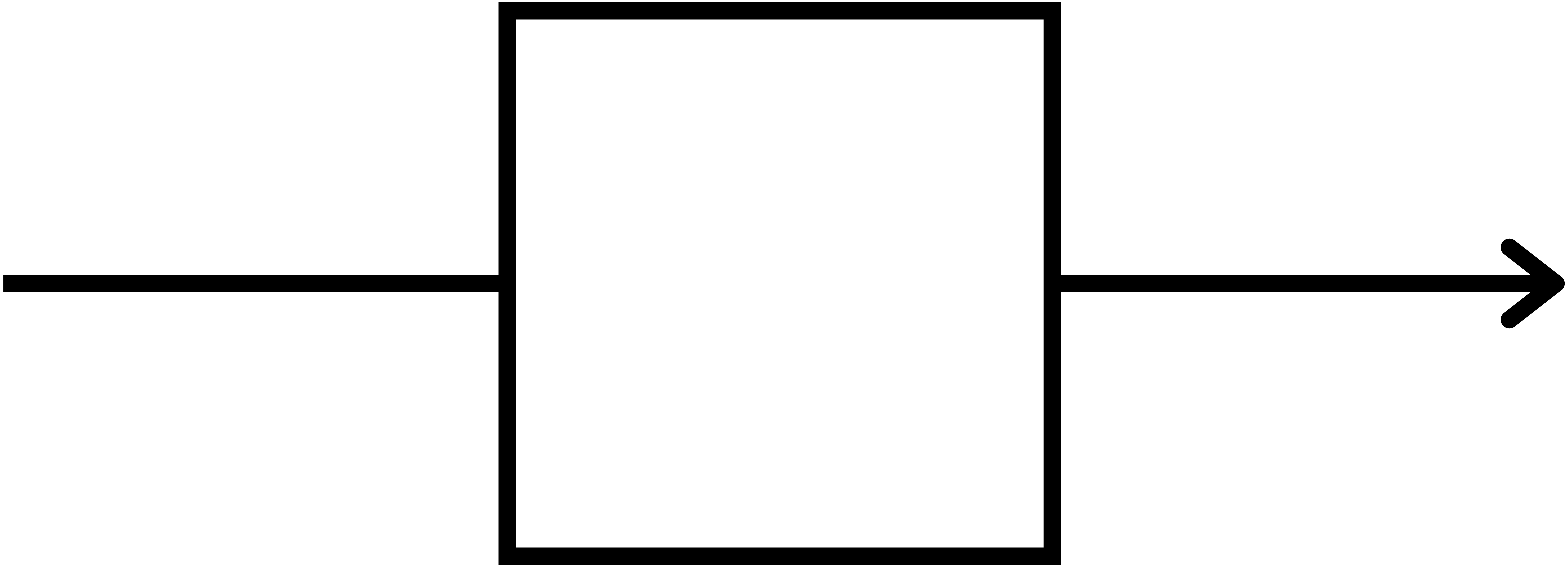


What is model-based machine learning?



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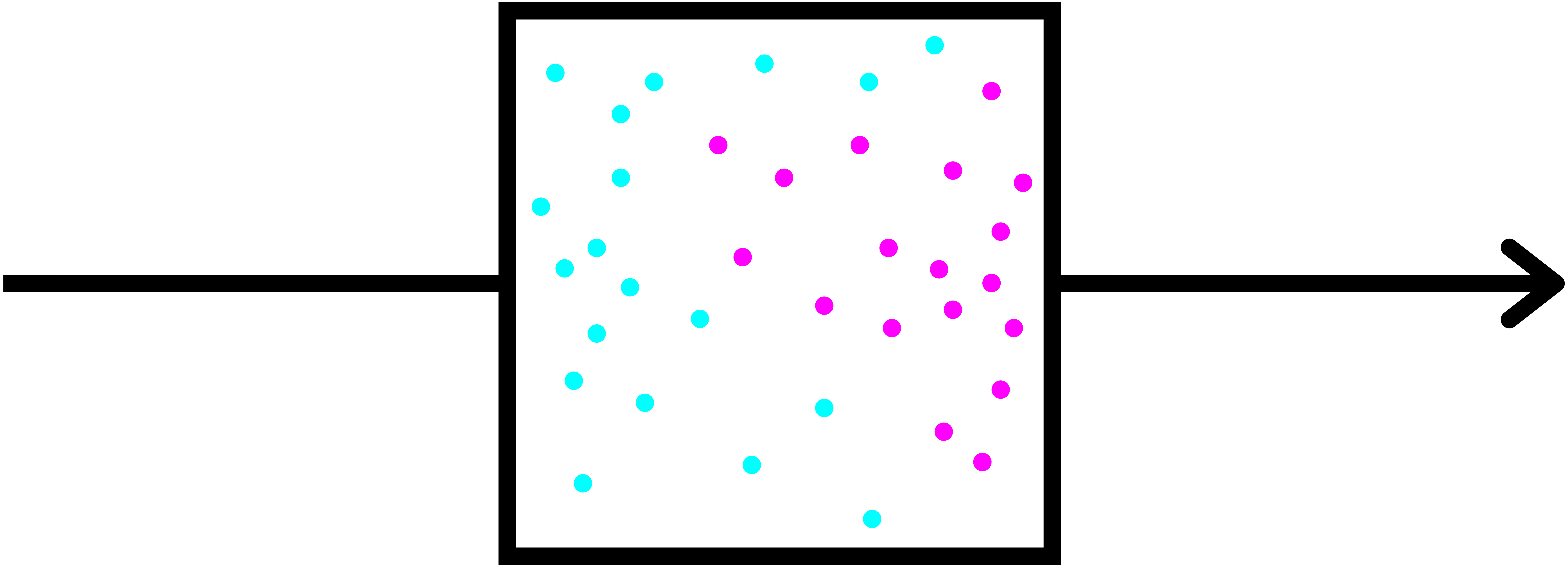

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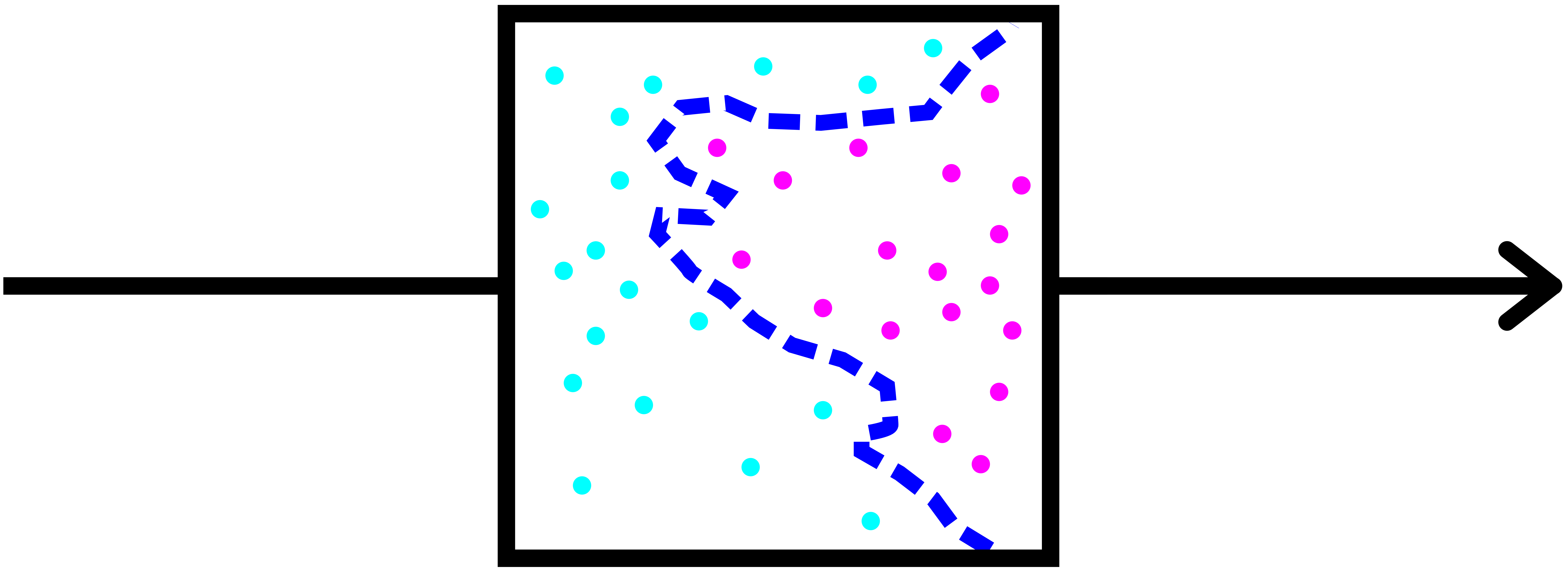

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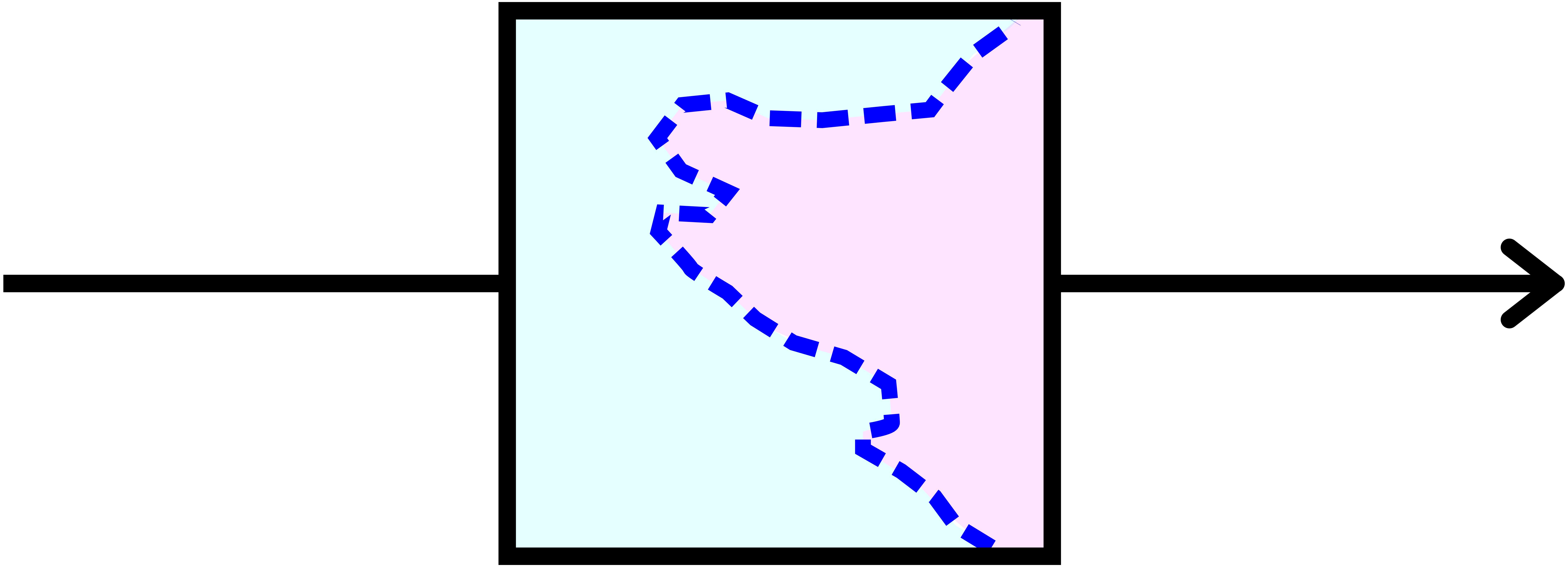
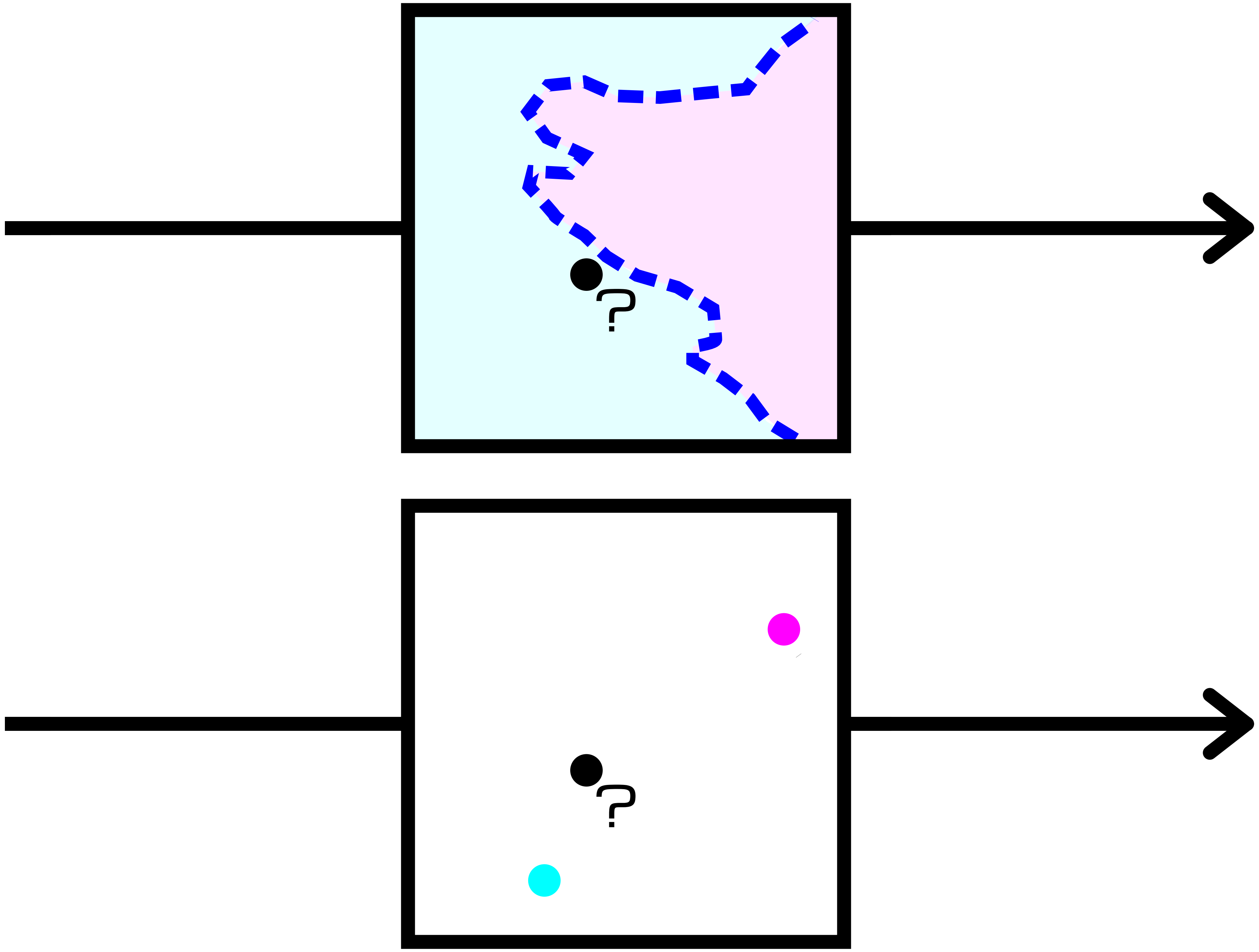


M.L. vs D.B. - what is the difference?



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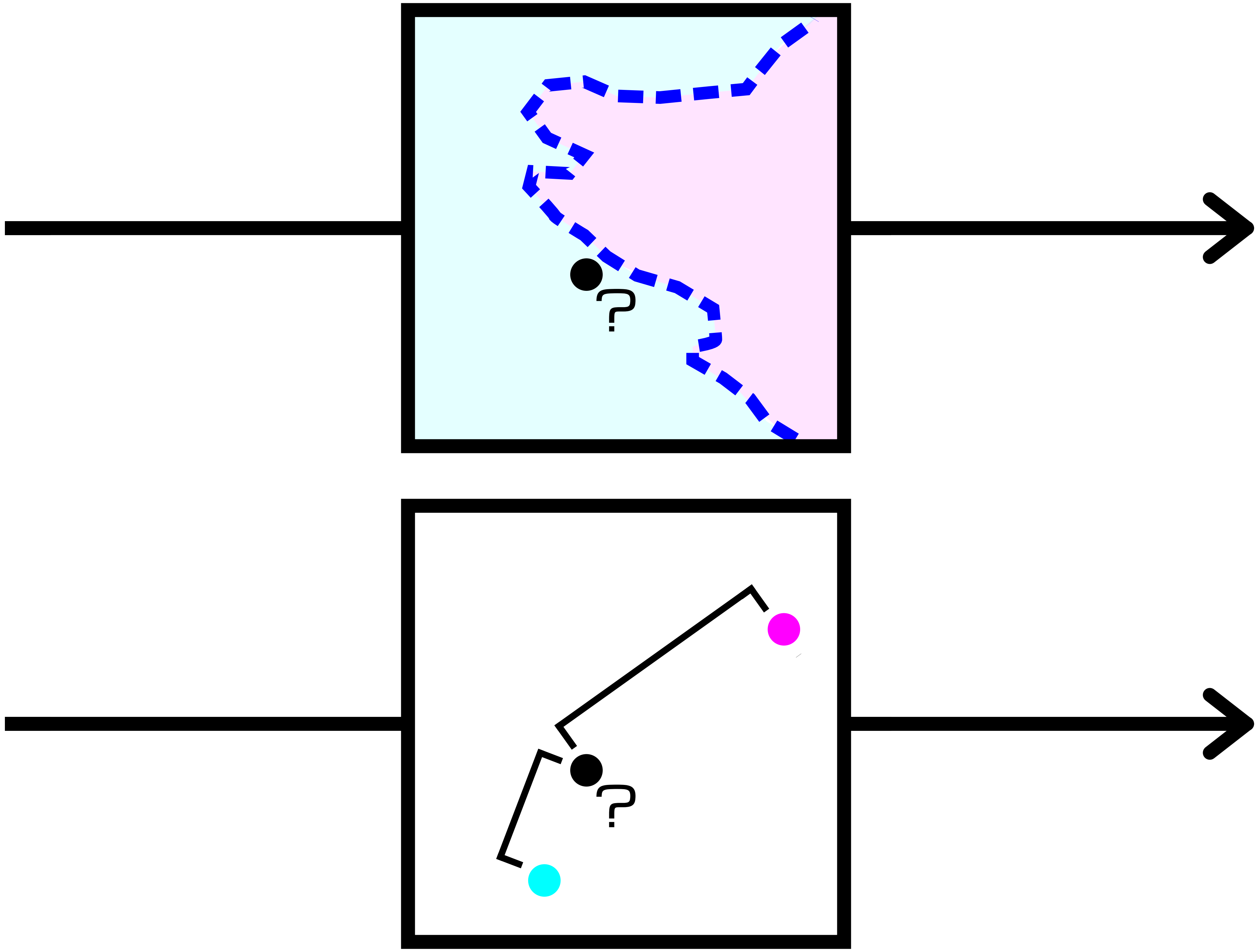
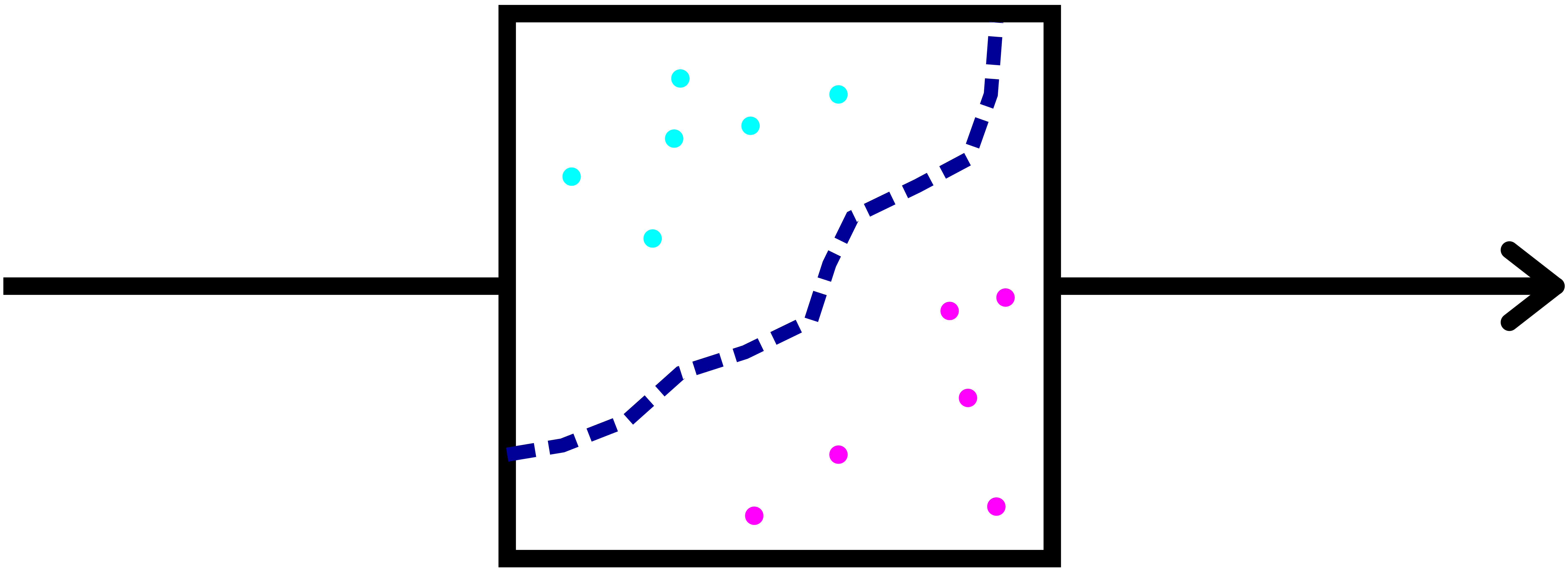


What are the key implications?



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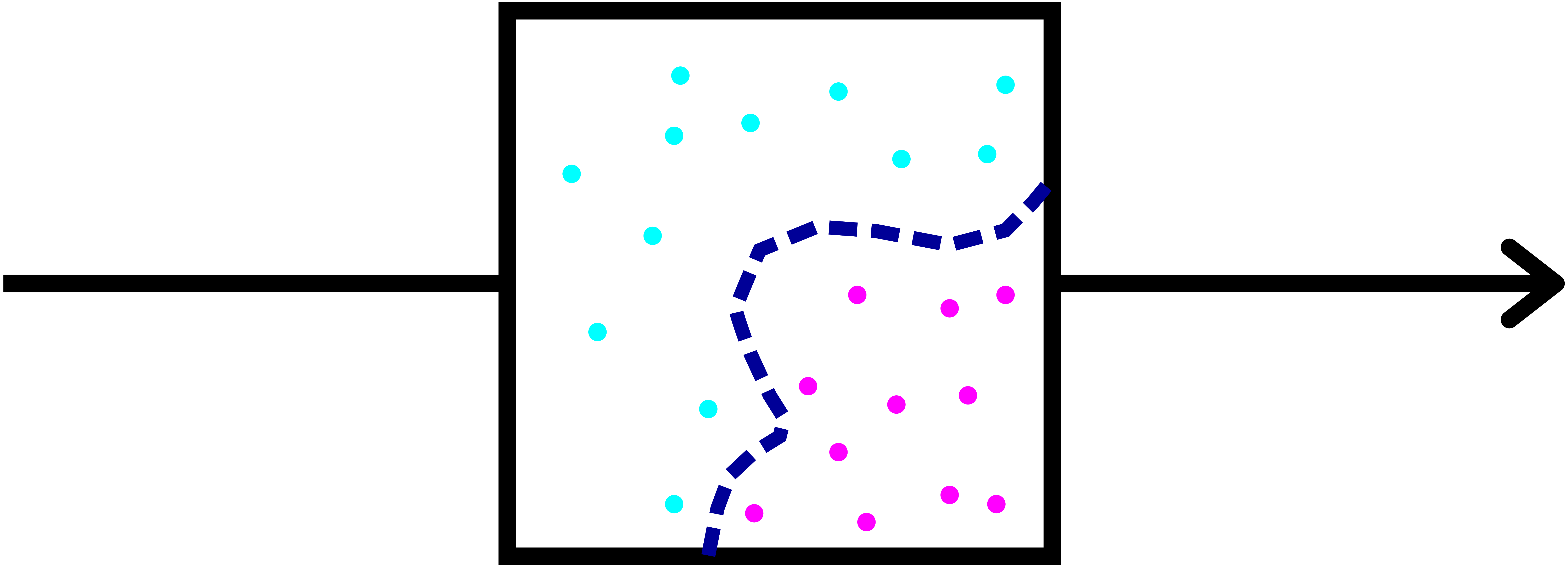

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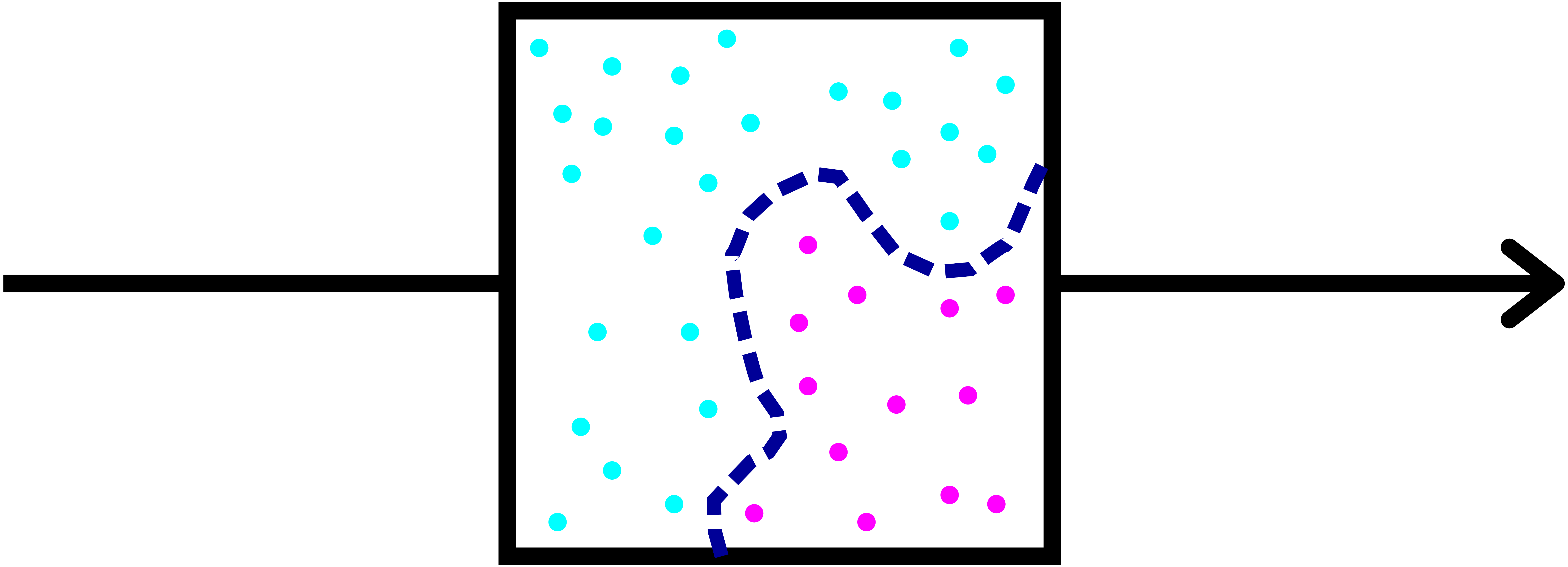

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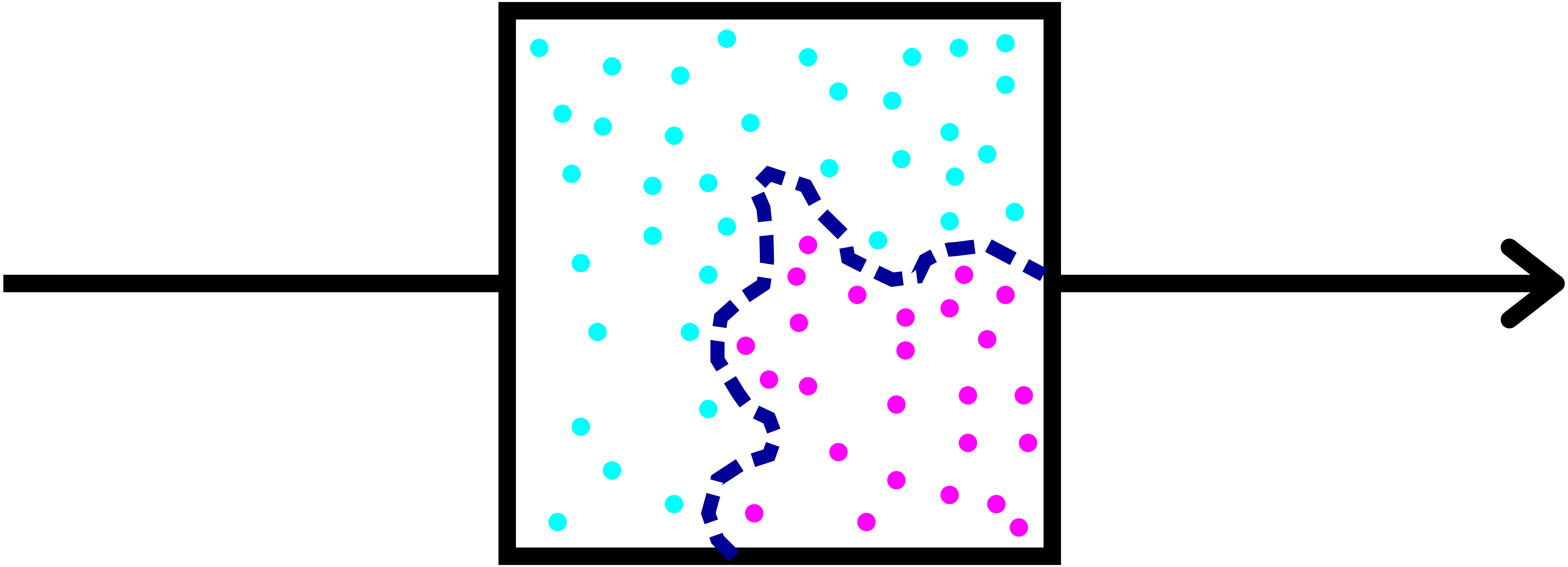

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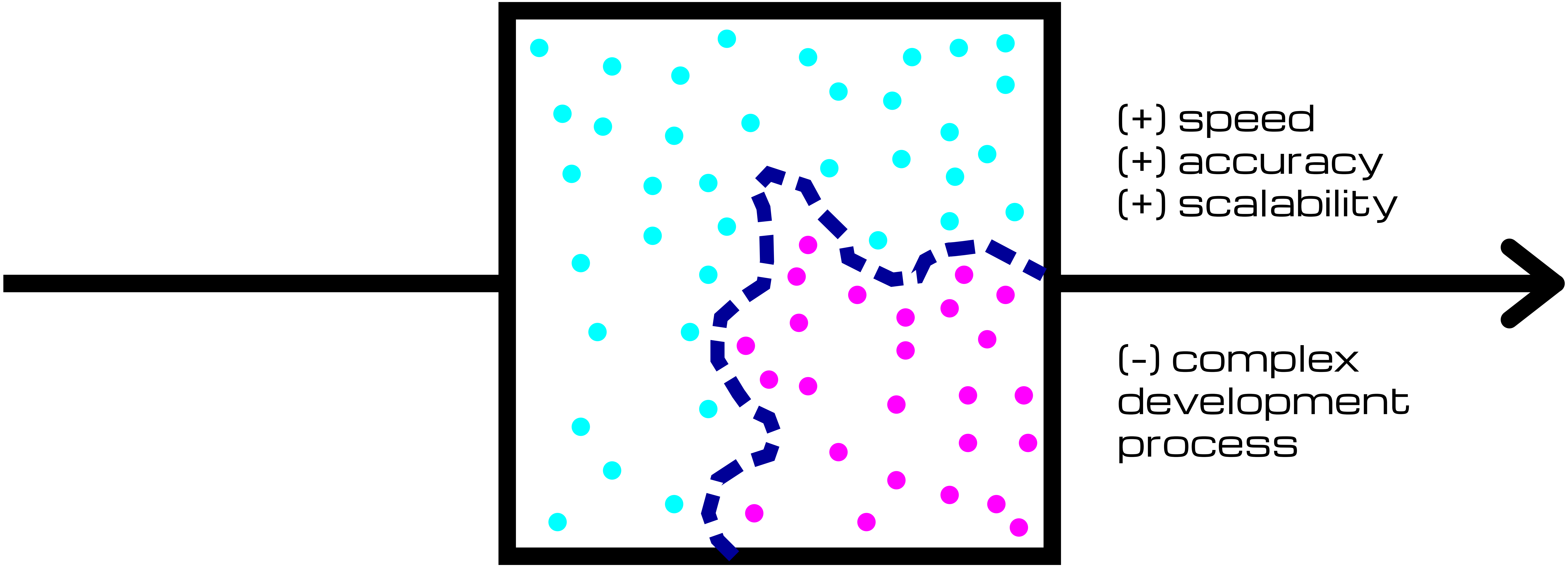
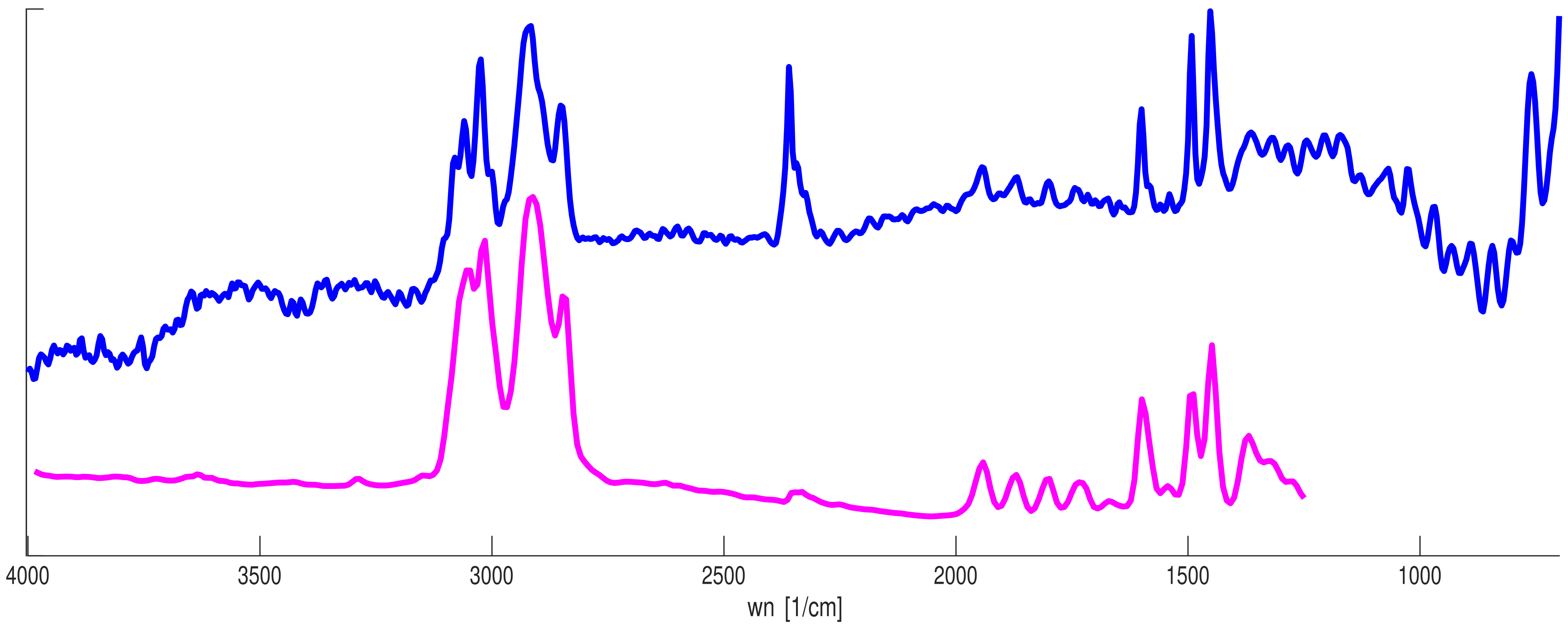


(+) speed
(+) accuracy
(+) scalability

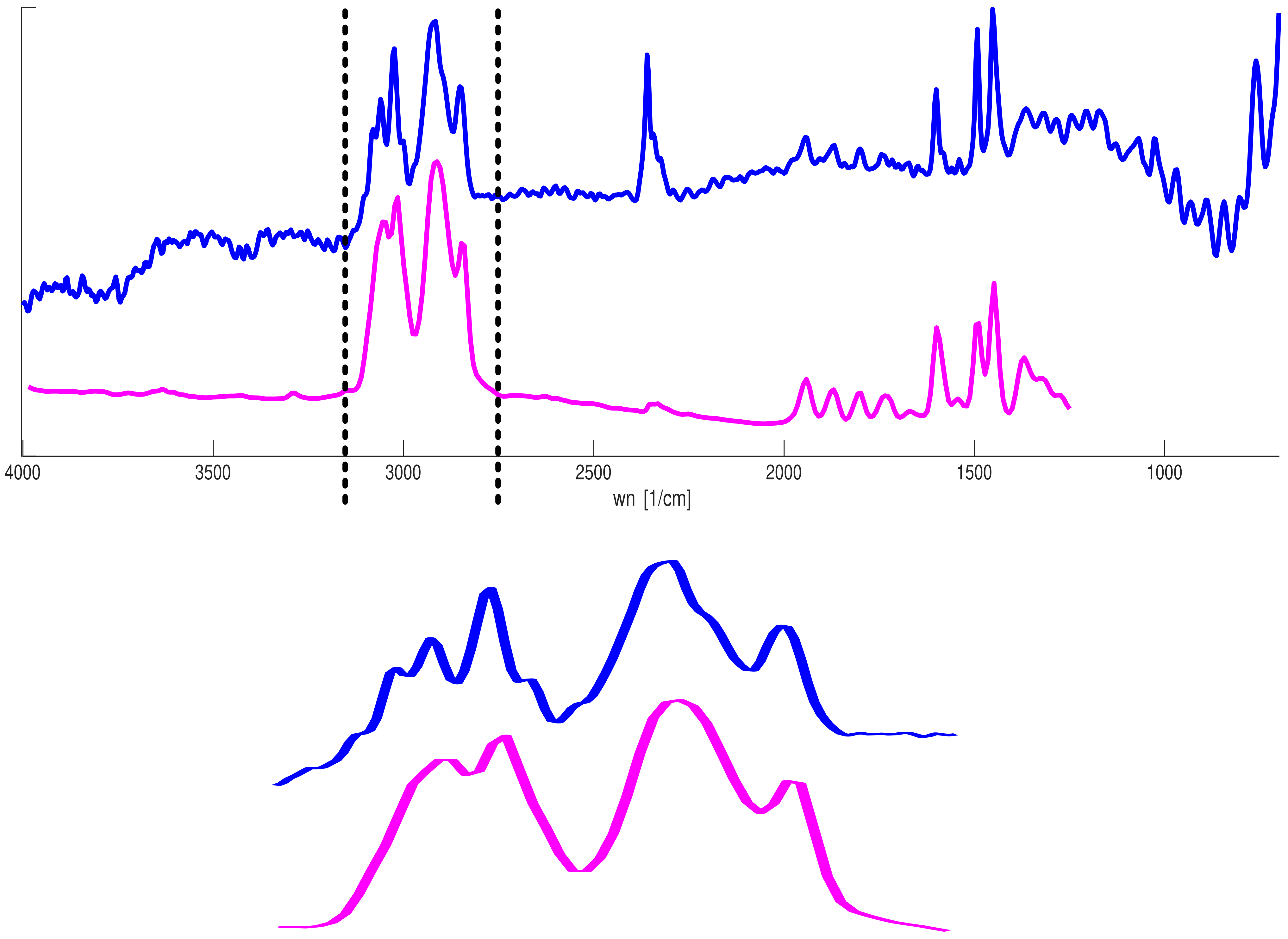
(-) complex development process

Building data-agnostic approaches

Spectra of different origin



Spectra of different origin



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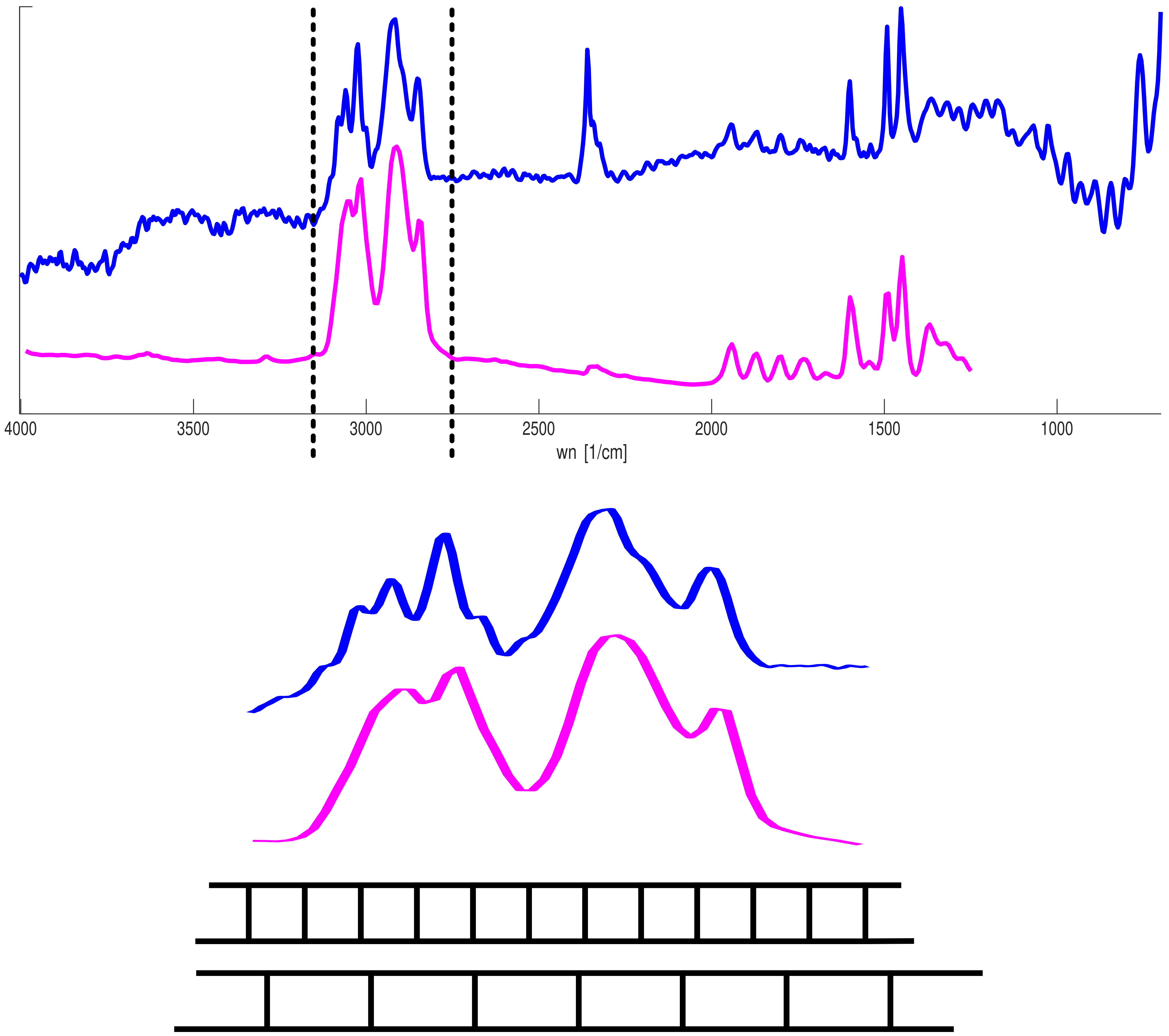

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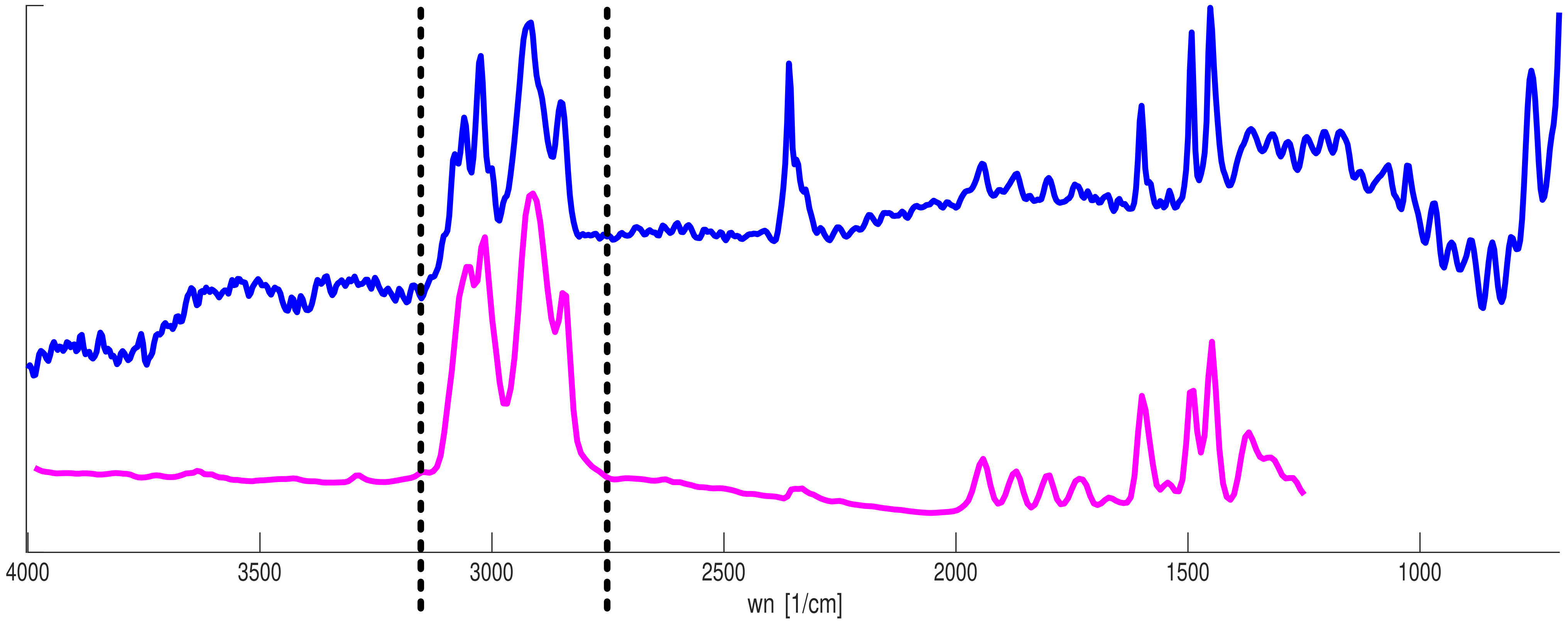

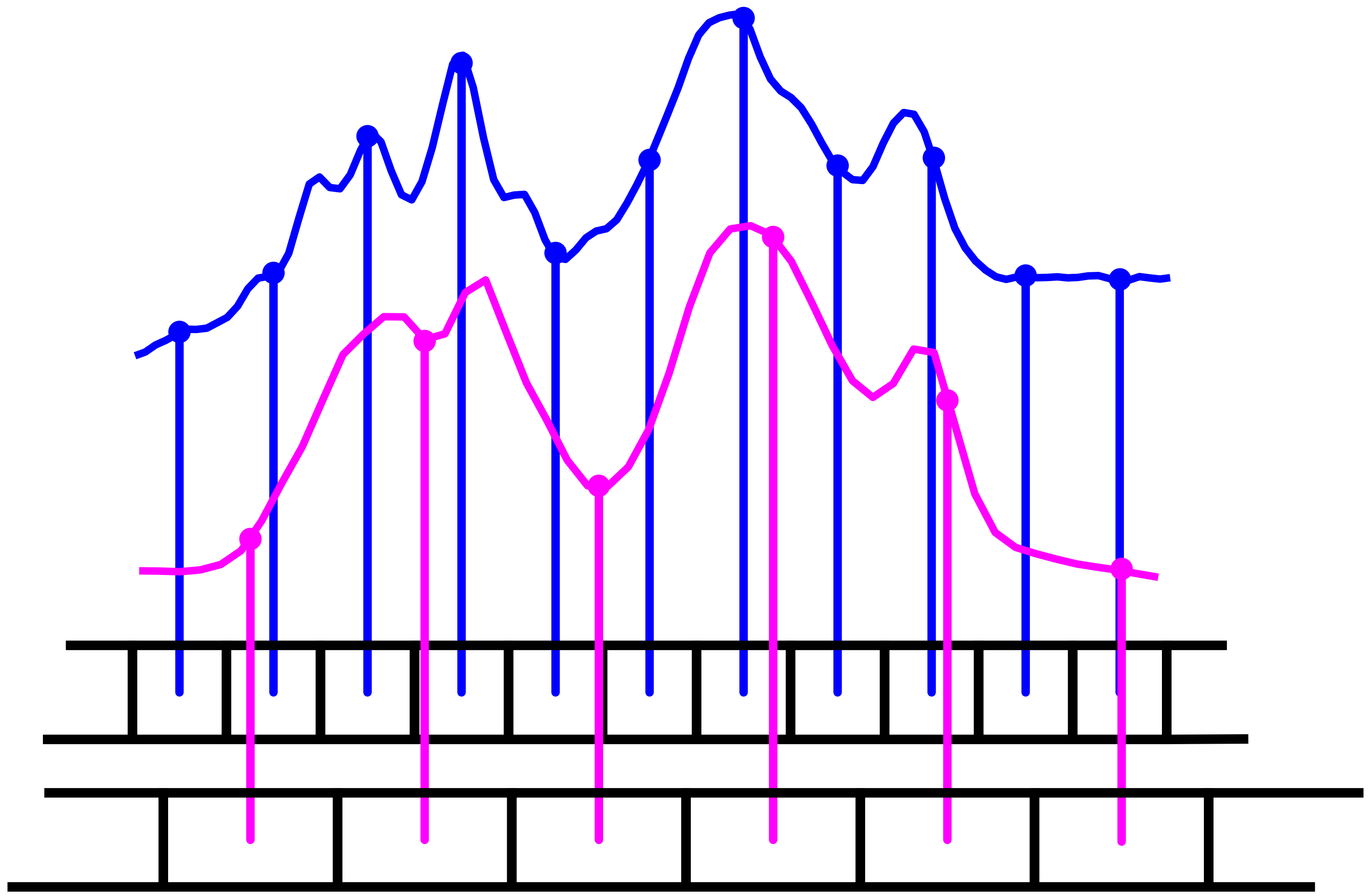

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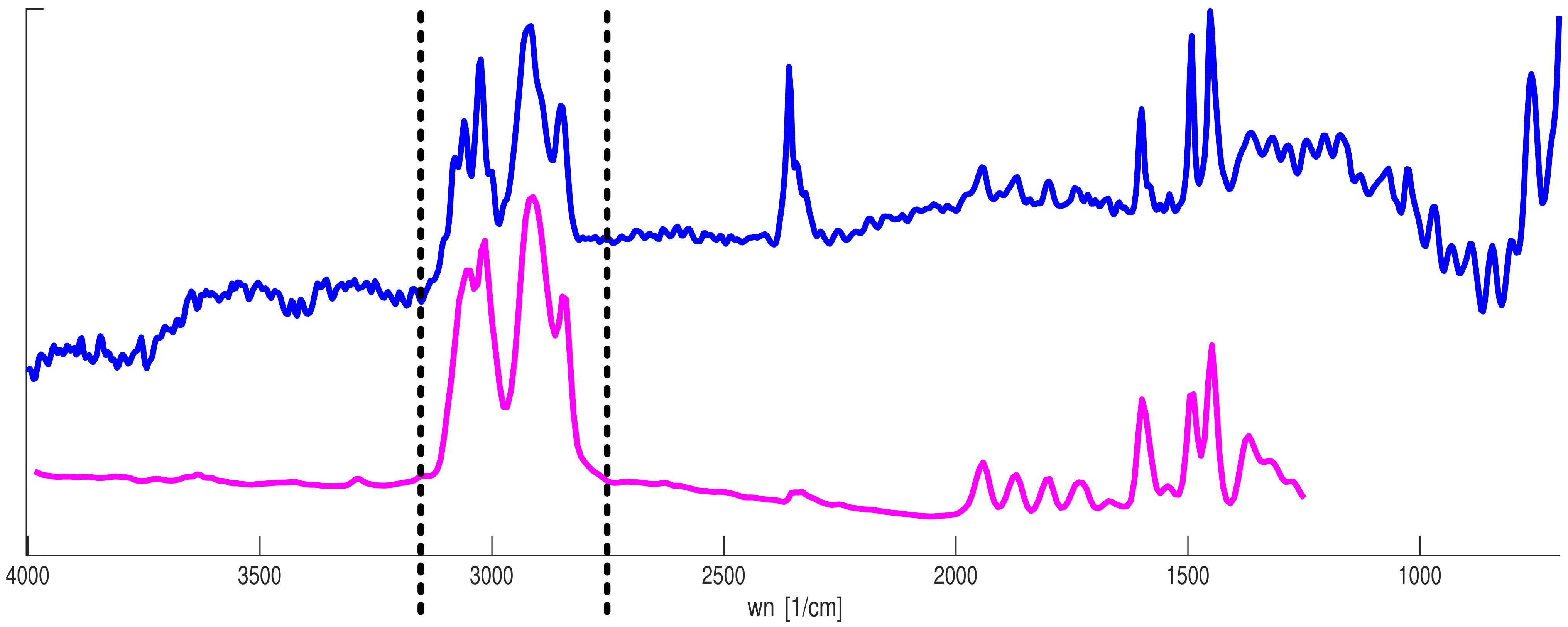
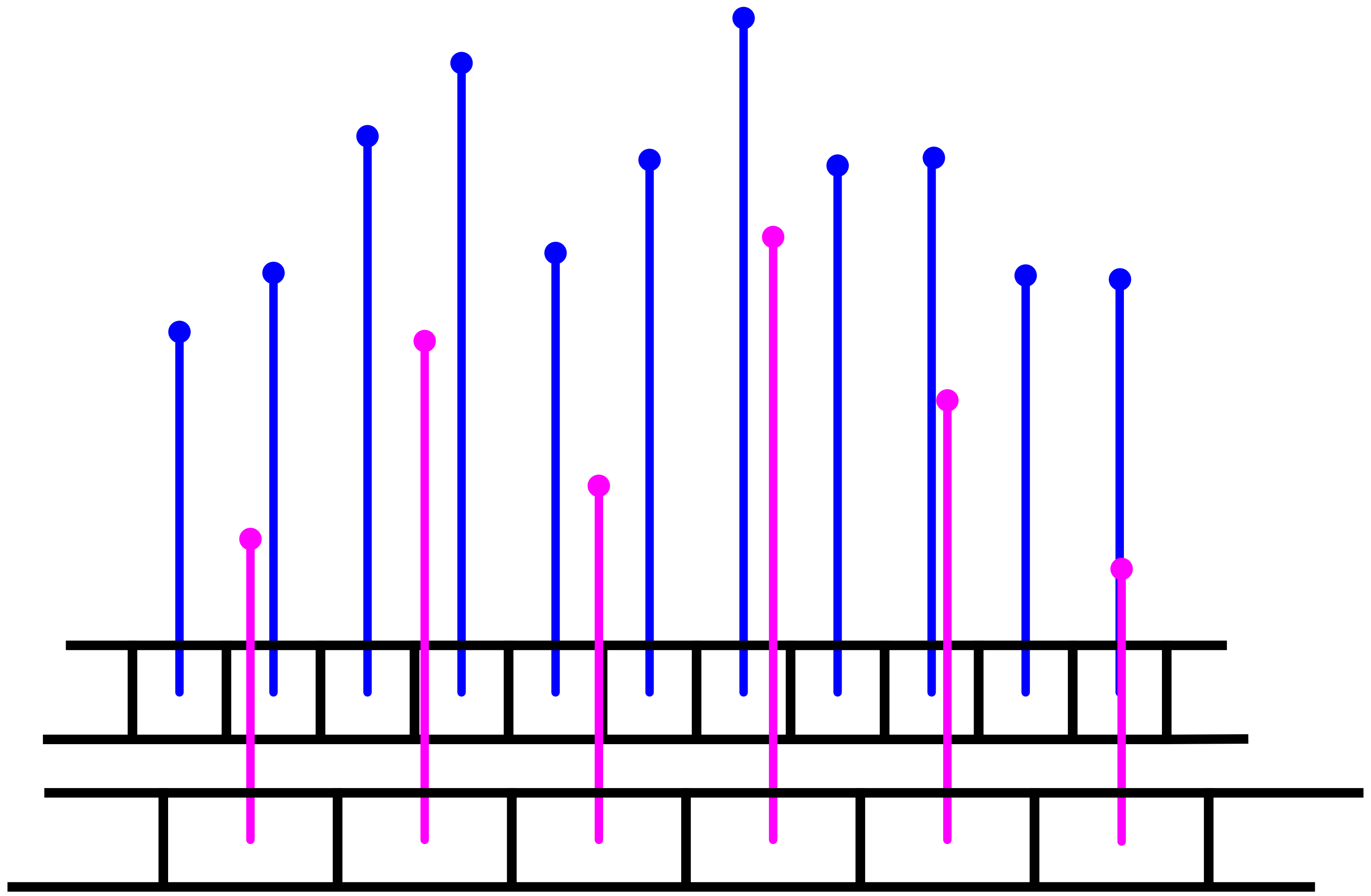




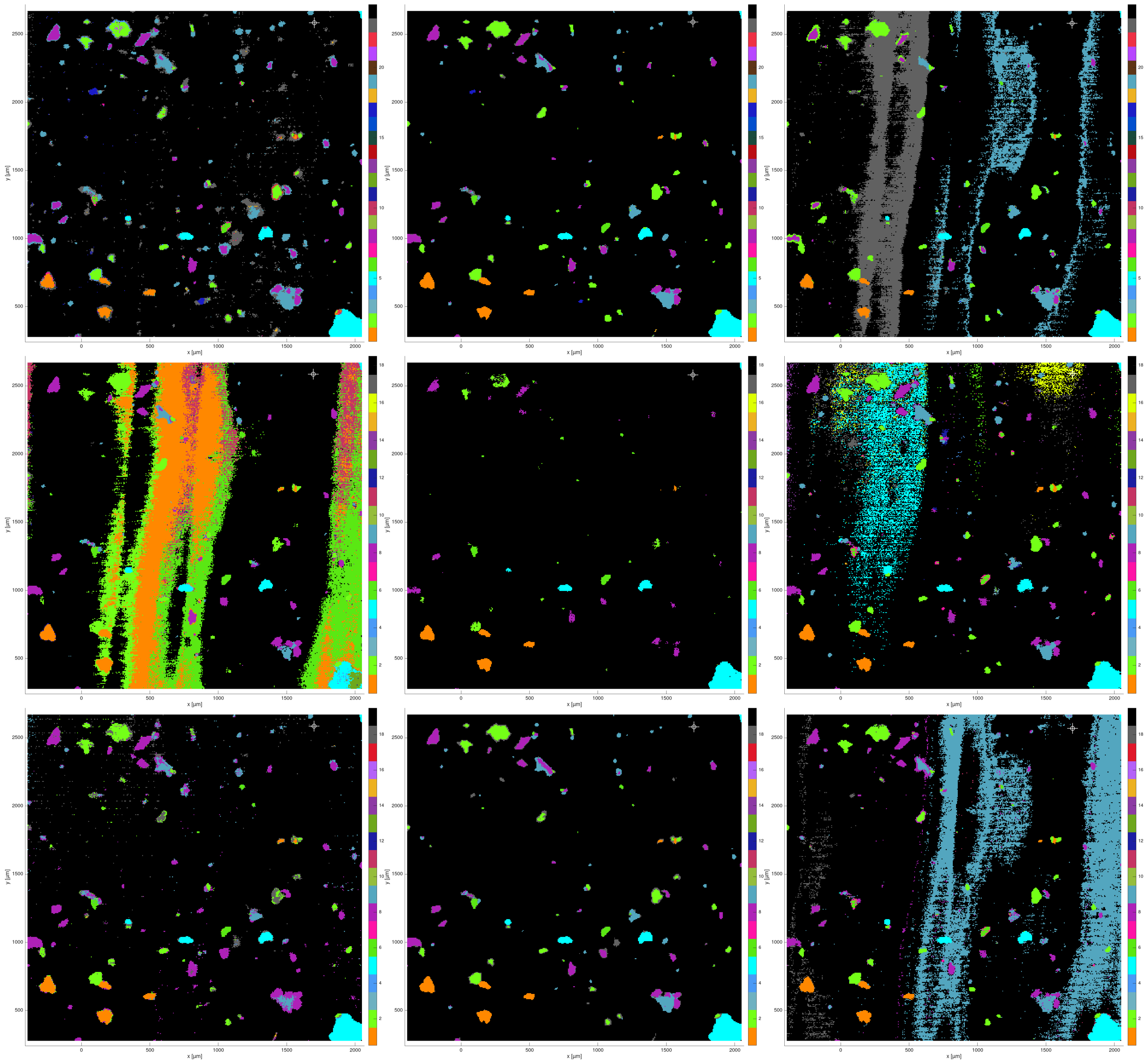
A comparison of different models

ANN | RF | DB

T1
4760 spectra,
4 [1/cm]
silicon wafer

T2
1720 spectra,
8 [1/cm]
Anodisc

T3
6980 spectra,
4 [1/cm]
Anodisc



A comparison of different models

RF | PP | PE | PET | PS

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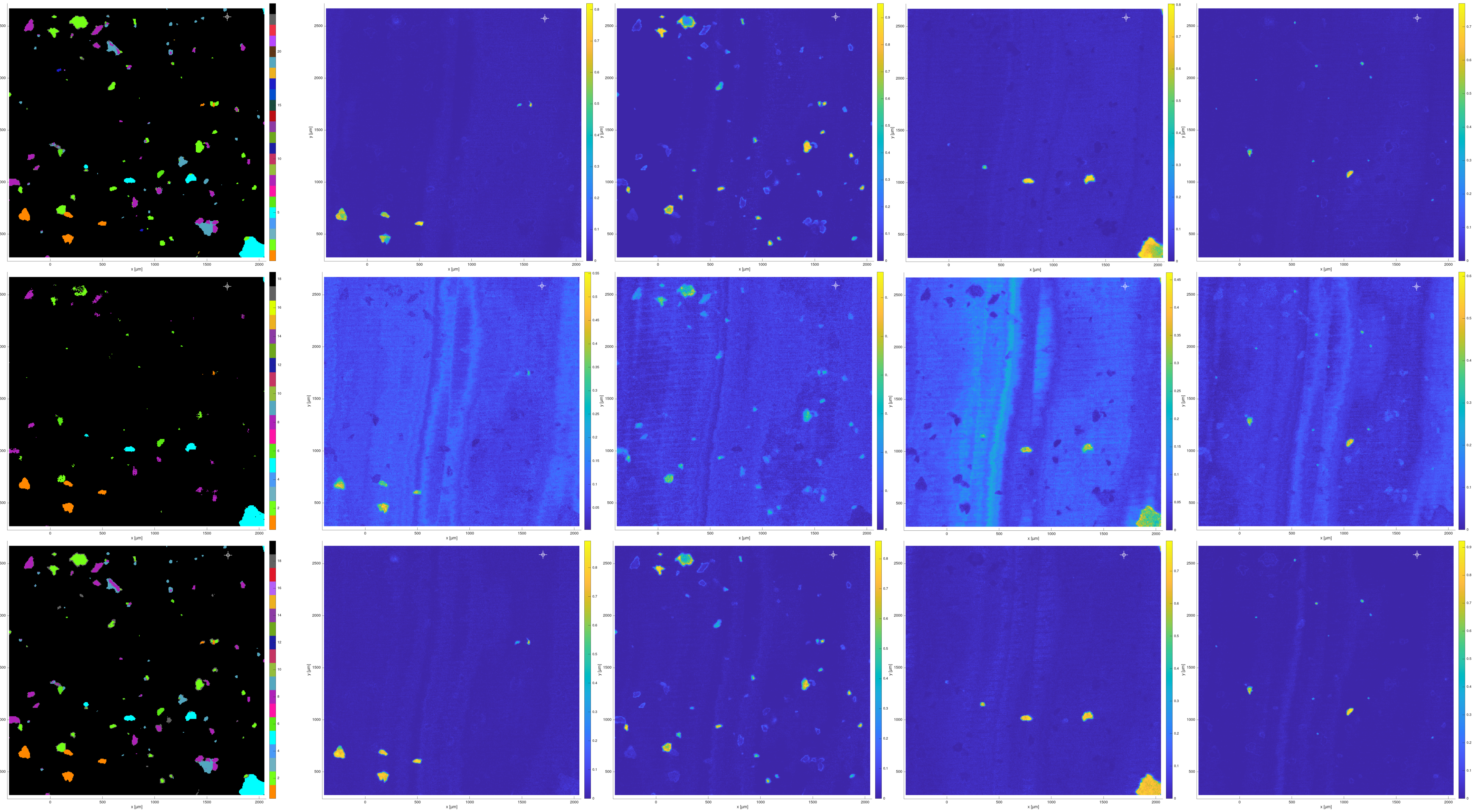
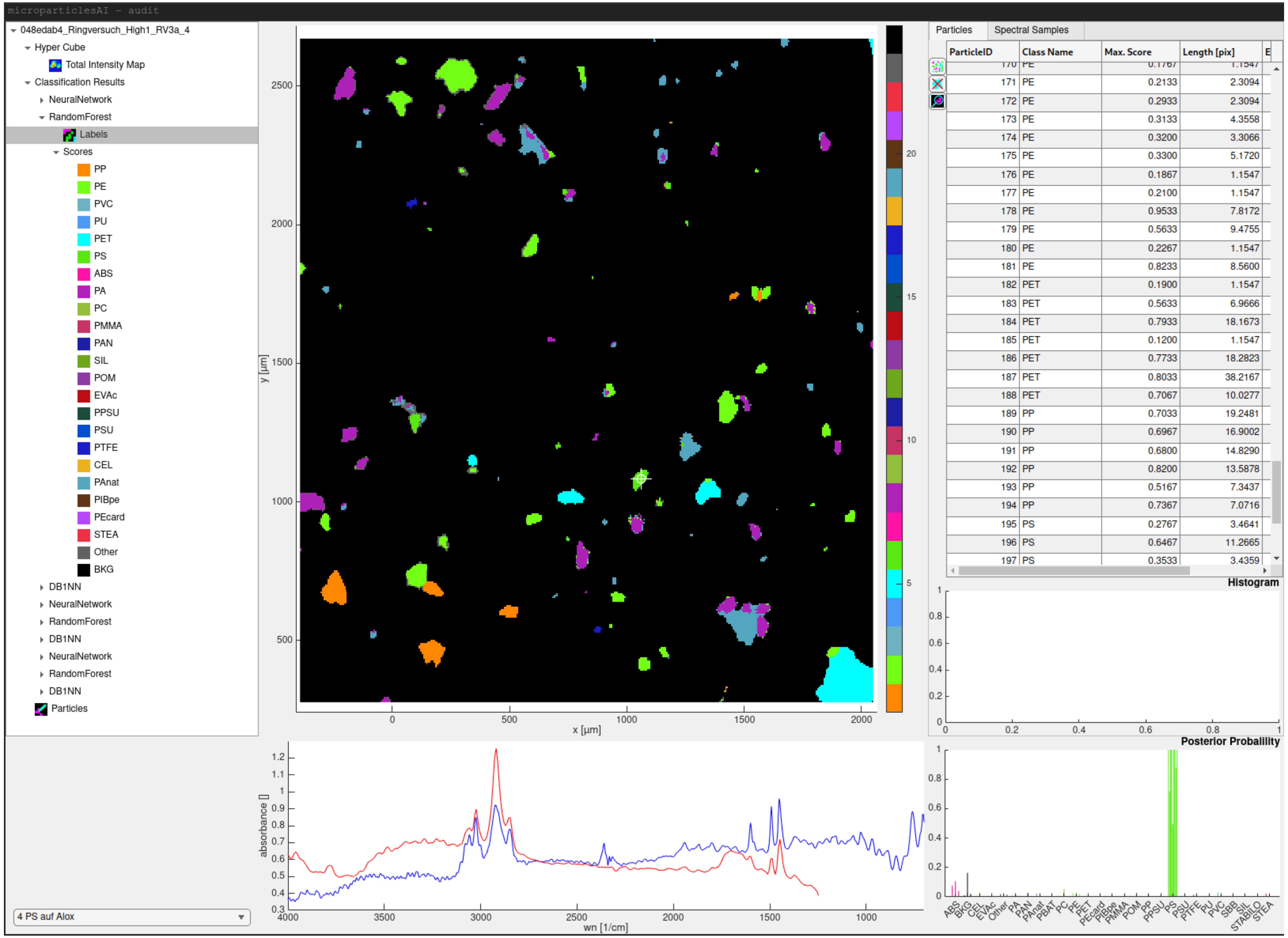


microparticlesAI (M-Engine)



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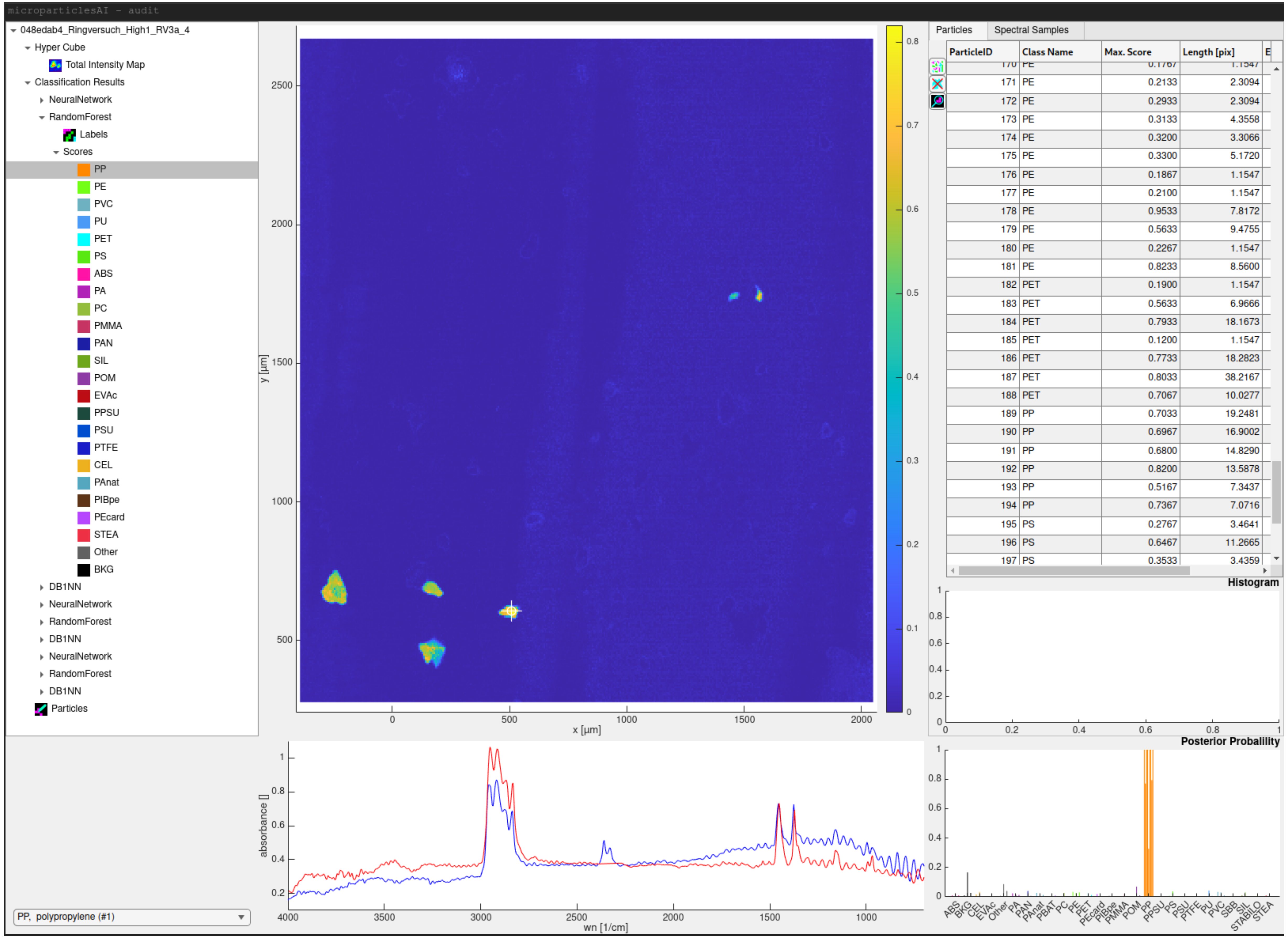

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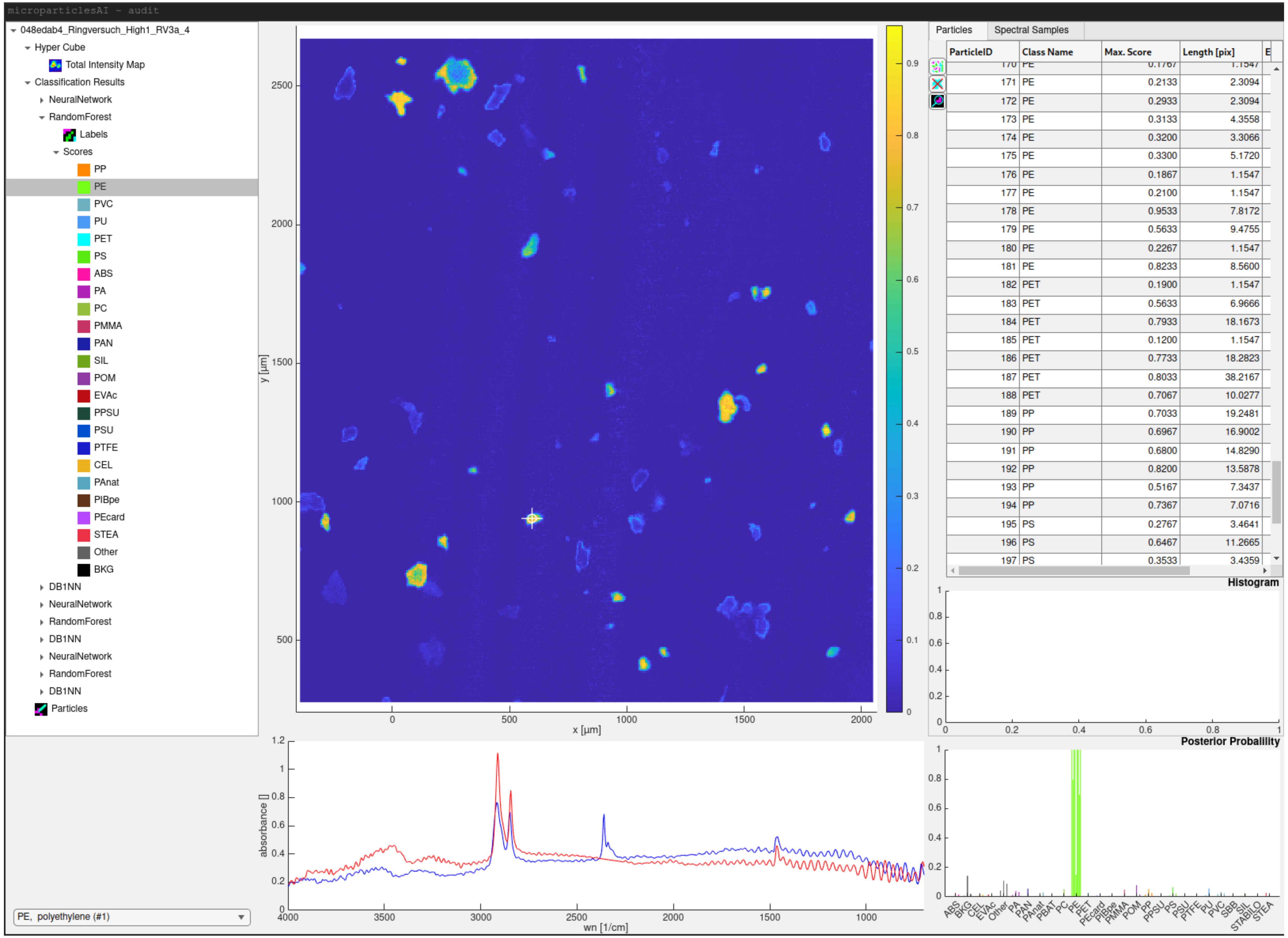

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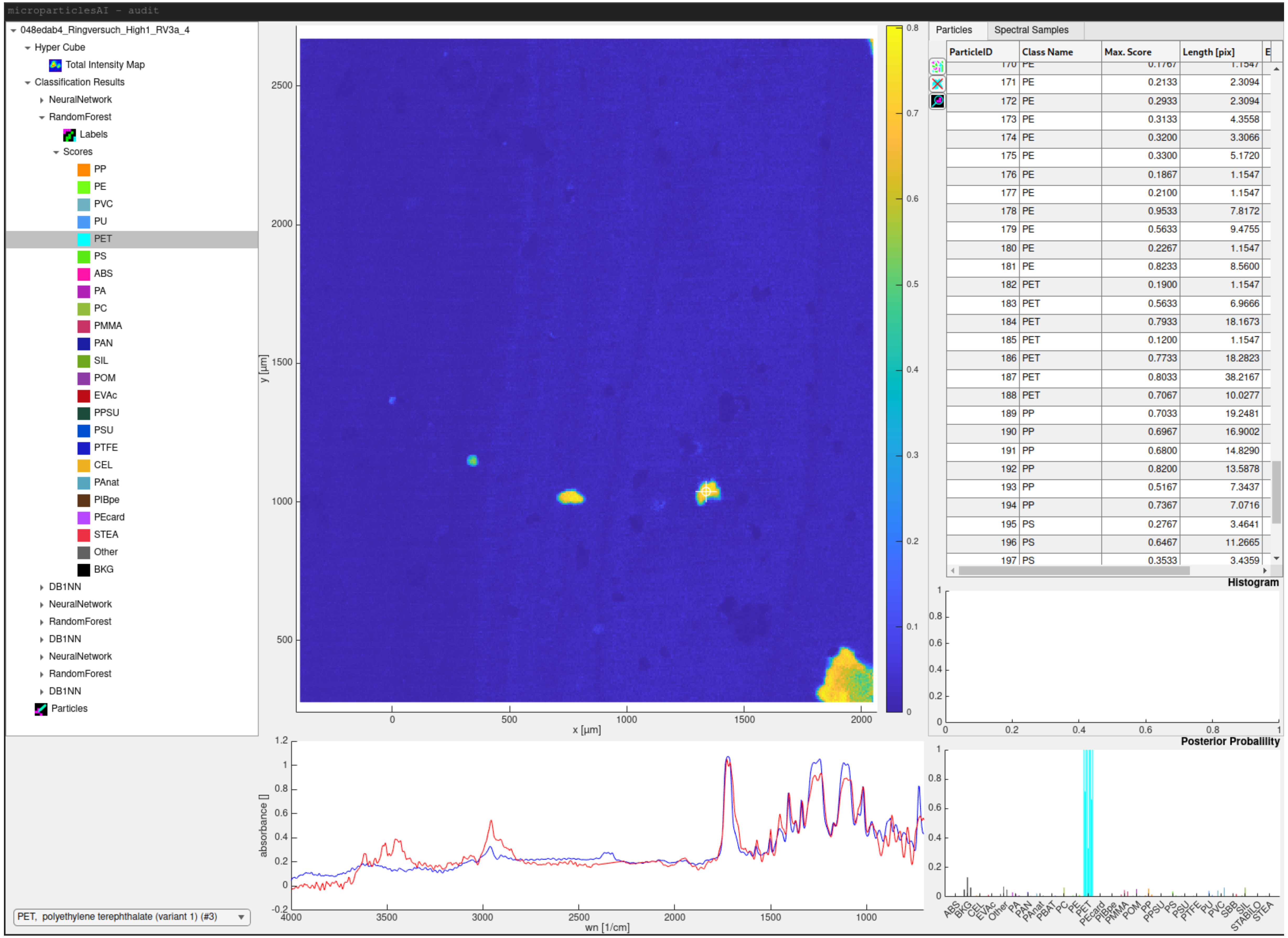

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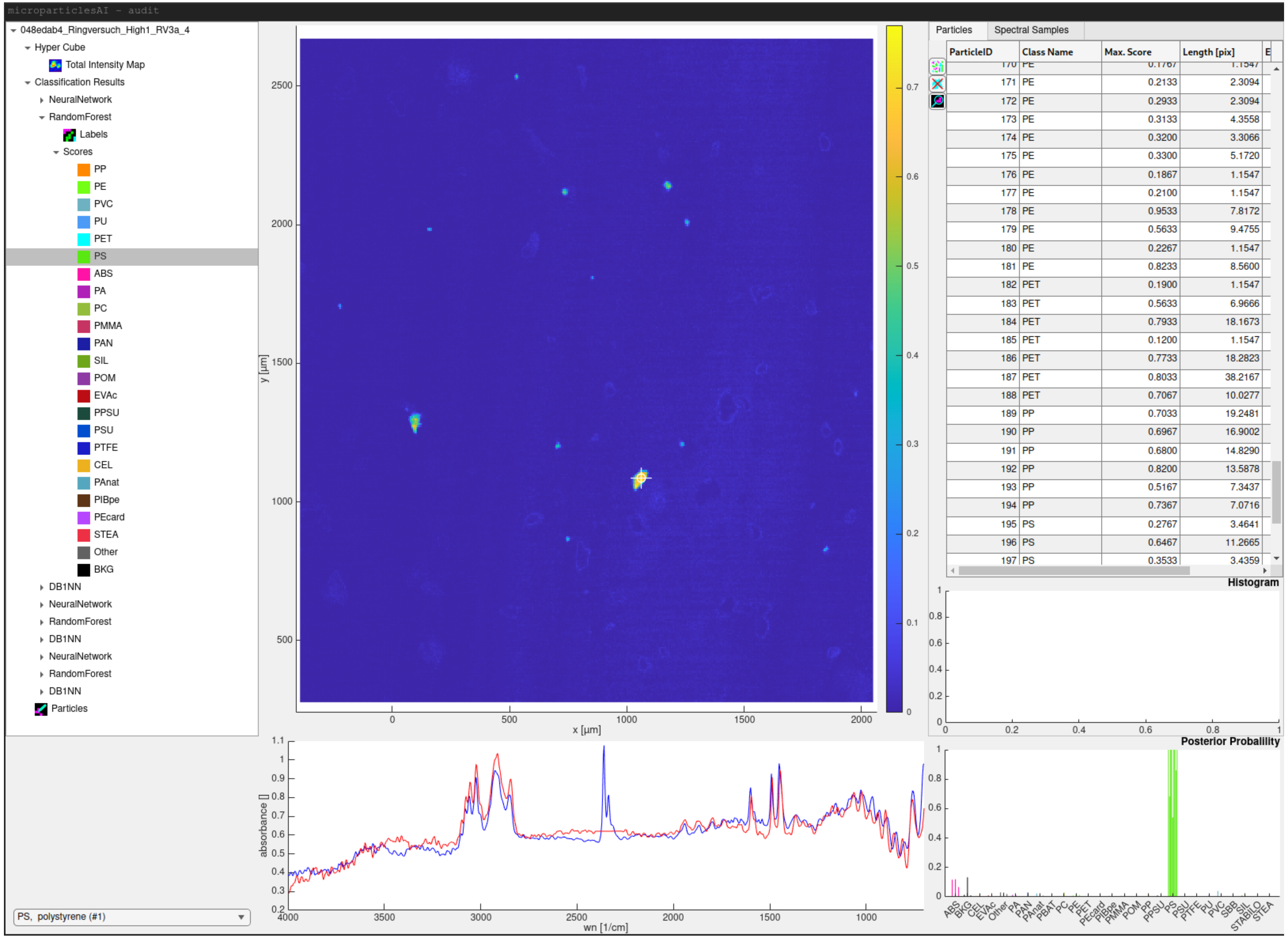

Compare and Validate Machine Learning Models

Definitions vs. talking in terms of data

Definitions vs. talking in terms of data

I consider FTIR spectra as polypropylene, which have a shoulder at 2875 cm-1, and the asymmetric and symmetric in-plane C-H (-CH3) at 1455 cm-1, as well as a shoulder at 1358 cm-1. There is also a peak at 1376 cm-1 which is assigned to the -CH3 group.

Considering scattering effects and total absorption the following effects will change the appearance of the spectrum:

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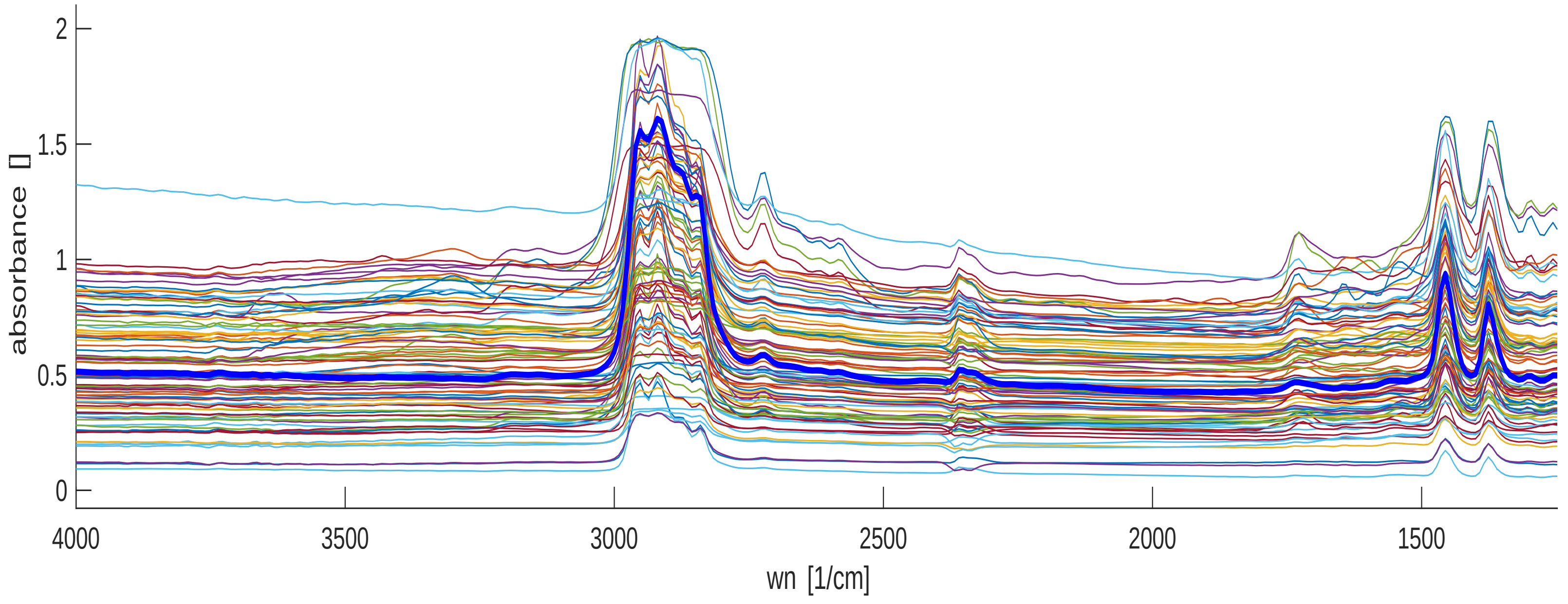
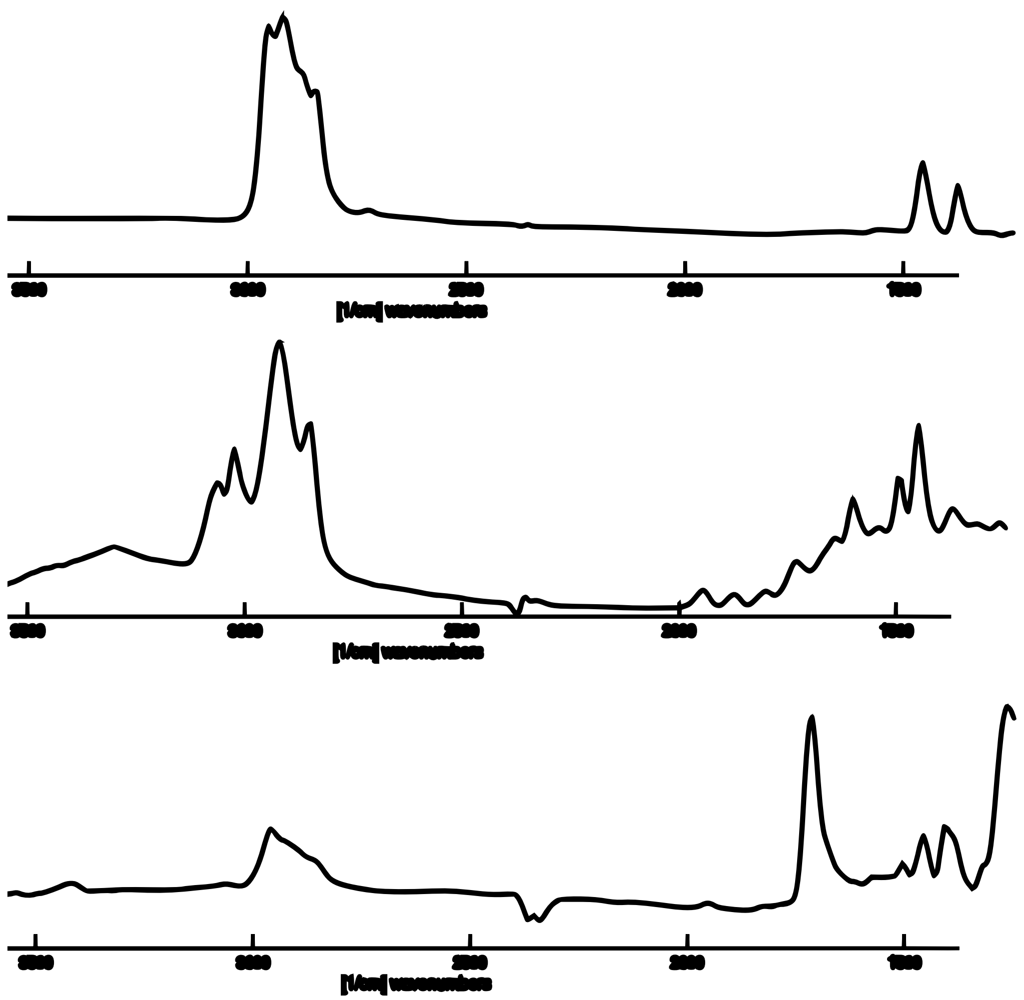


ISO 24187:2023 Evaluation / Validation

$\vec{x}$ | y



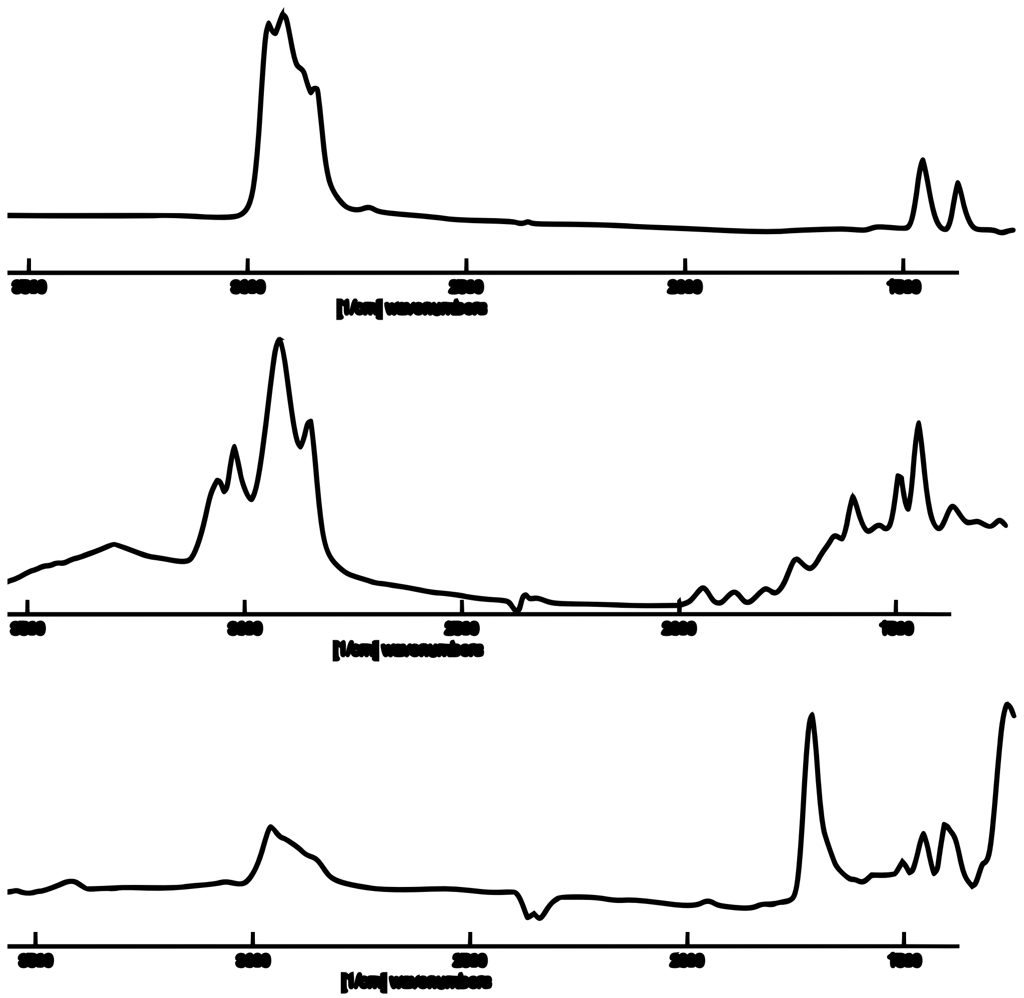
PP

PS

PET

ISO 24187:2023 Evaluation / Validation

$\vec{x}$



y	$\hat{y}$	
PP	PP	✓
PS	PS	✓
PET	PBT	✗

ISO 24187:2023 Evaluation / Validation

Expert (y)

	PP	PE	PS	PA	PC	PVC	PMMA	PPSU	PU
PP									
PE									
PS									
PA									
PC									
PVC									
PMMA									
PPSU									
PU									

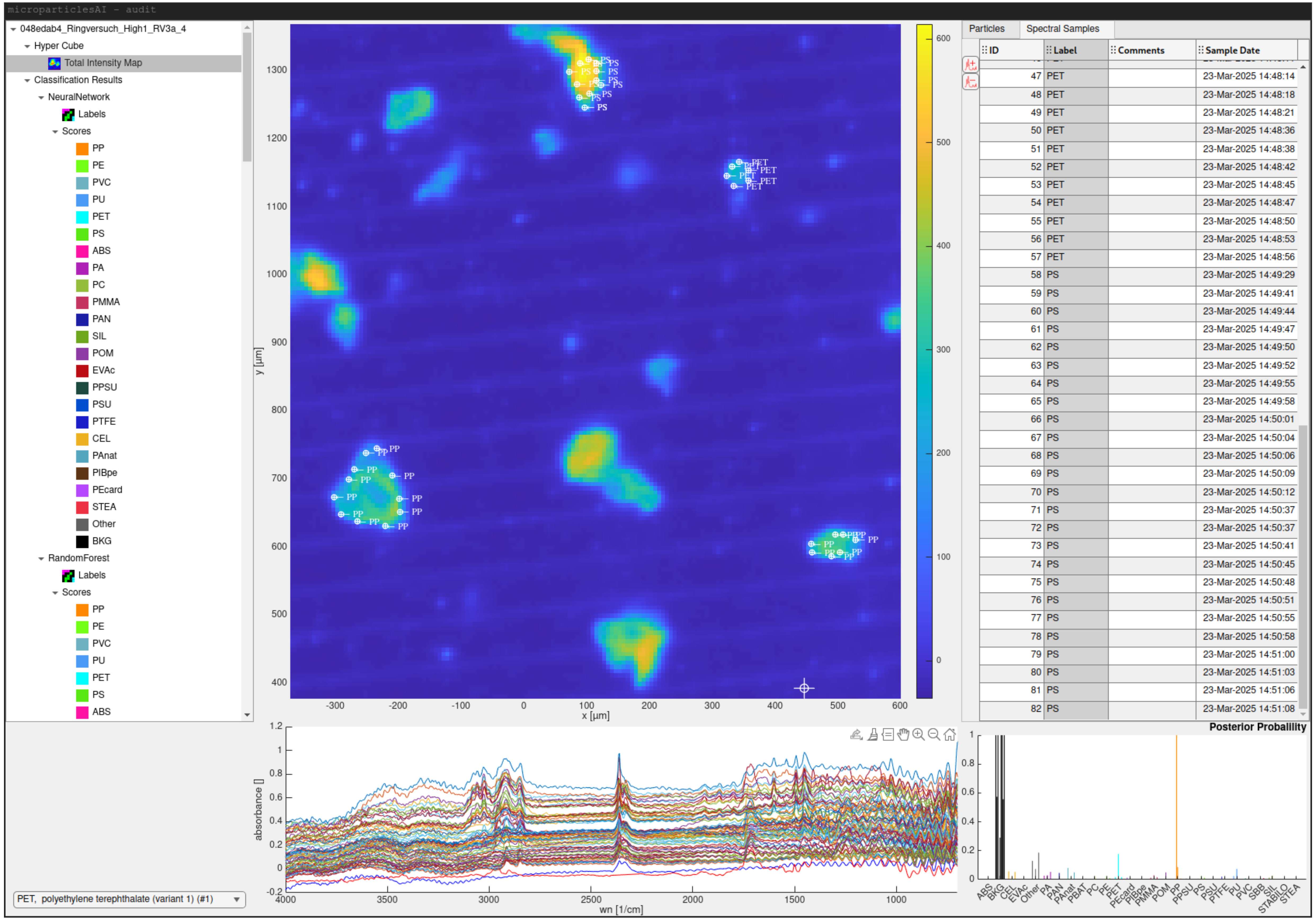
Predicted ($\hat{y}$)

ISO 24187:2023 Evaluation / Validation

Expert (y) / Predicted (ŷ)

Expert (y) \ Predicted (ŷ)	PP	PE	PS	PA	PC	PVC	PMMA	PPSU	PU
PP	46	12							
PE	15	31				1			
PS			89						
PA				22			3		
PC					14				
PVC					2	56			13
PMMA							33		
PPSU		1						36	
PU						17			95

Validate (app) for ISO 24187 validation



Validate (app) for ISO 24187 validation

Hufnagl Chemometrics Validate

File

Test Data | Assign Labels | Validation

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048edab4_Ringversuch_High1_RV3a_4-#3	PP	PosX: -270.0754 PosY :714.0796 orig comments:	048edab4_Ringversuch_High1_RV3a_4
048edab4_Ringversuch_High1_RV3a_4-#4	PP	PosX: -252.2999 PosY :738.5833 orig comments:	048edab4_Ringversuch_High1_RV3a_4
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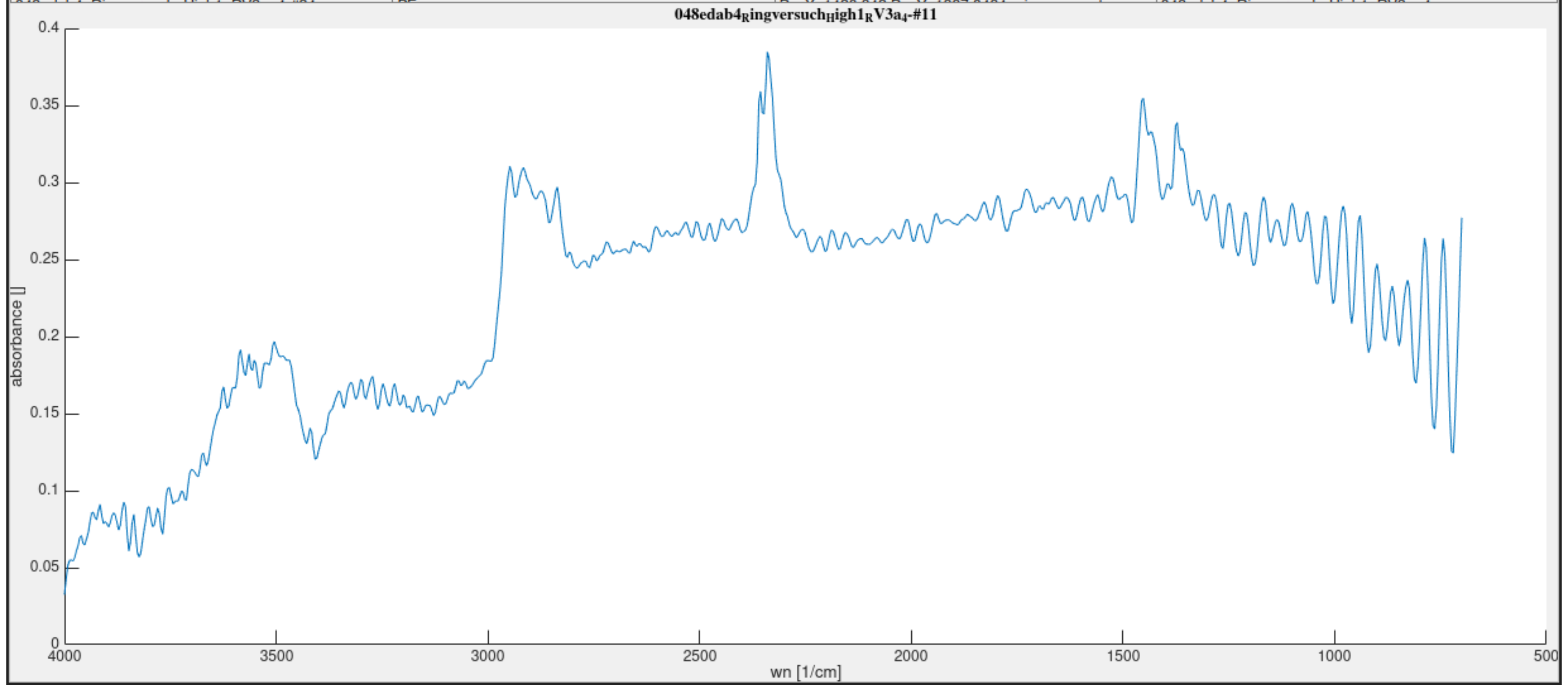
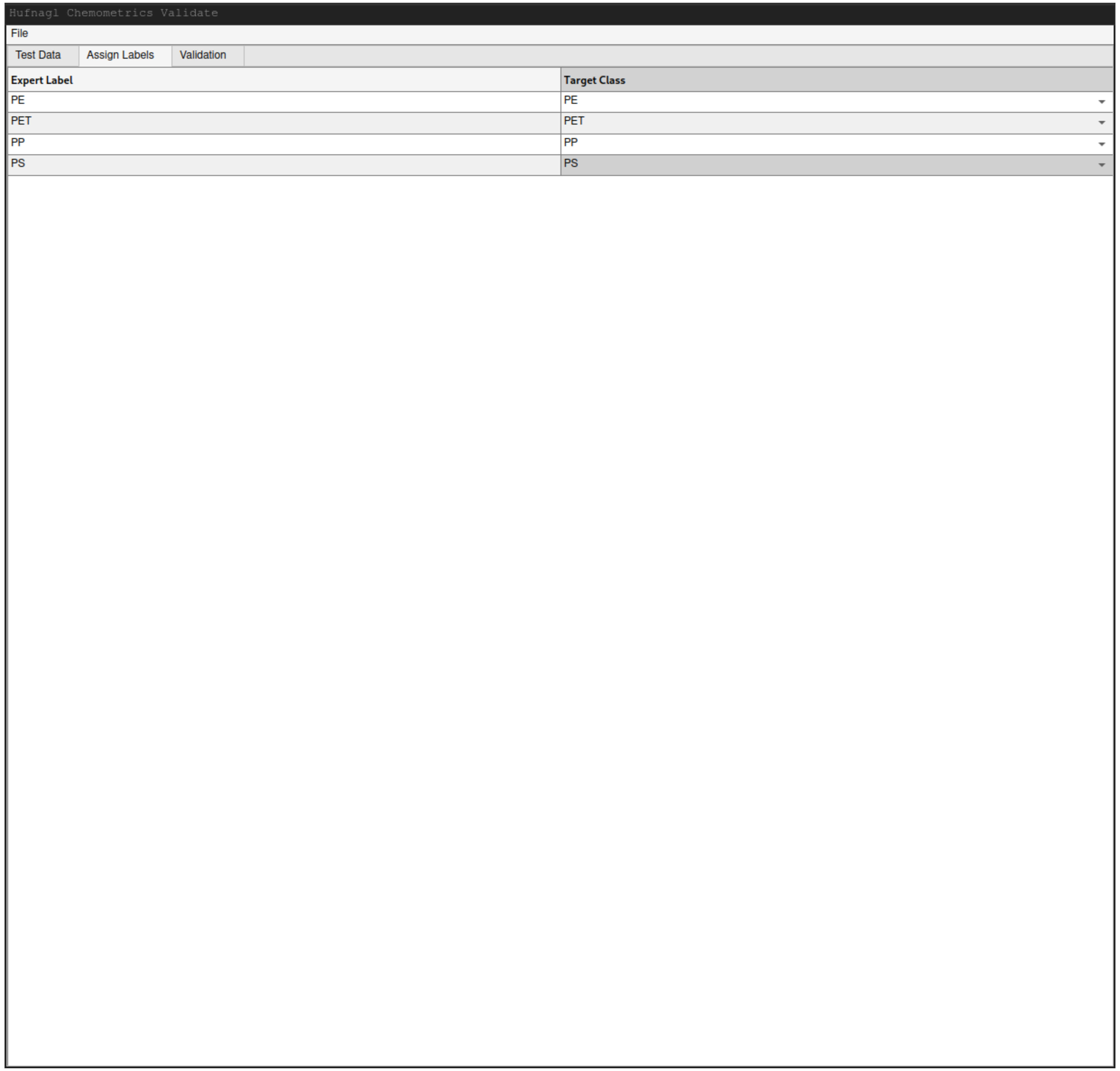


Validate (app) for ISO 24187 validation



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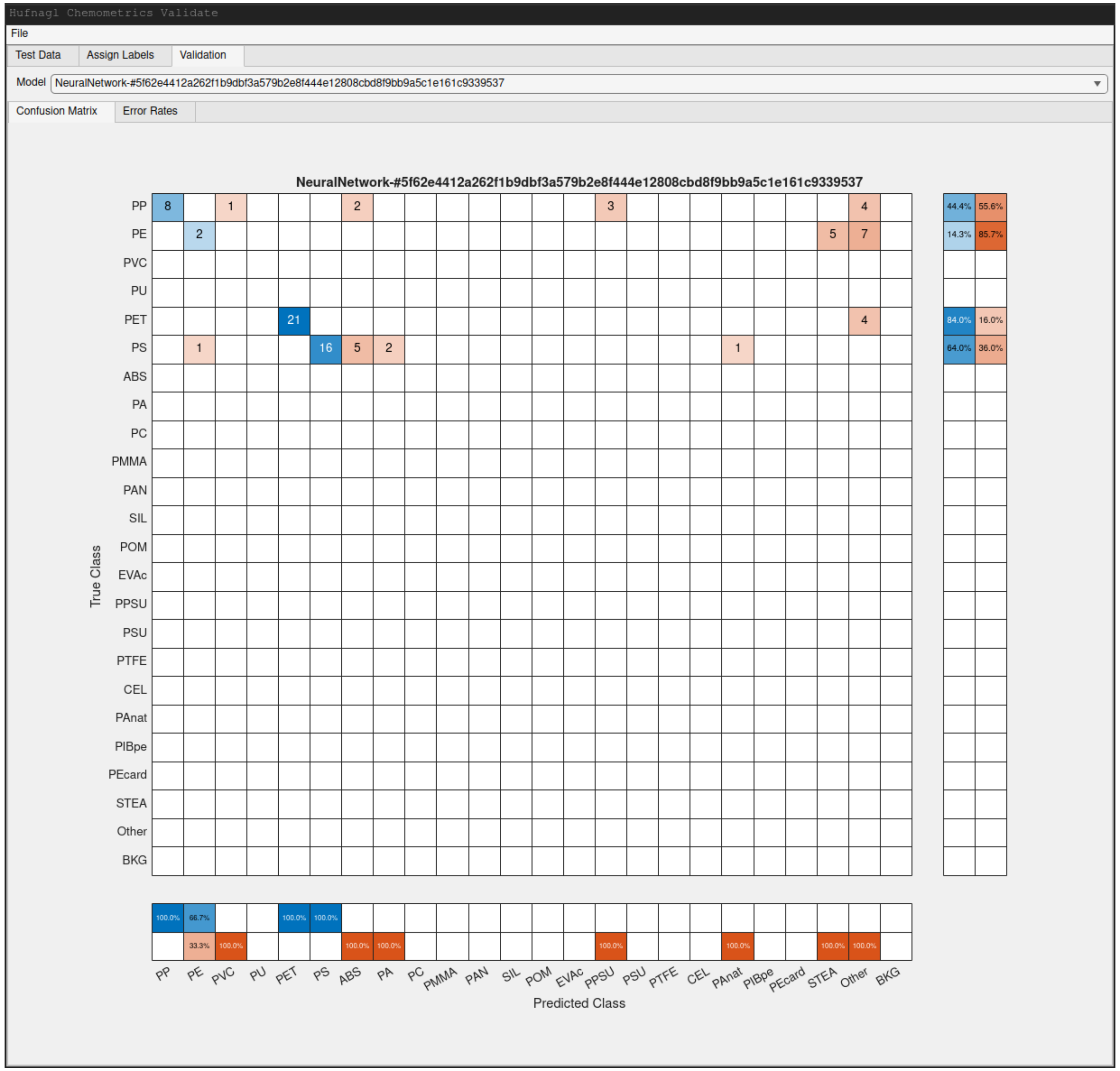

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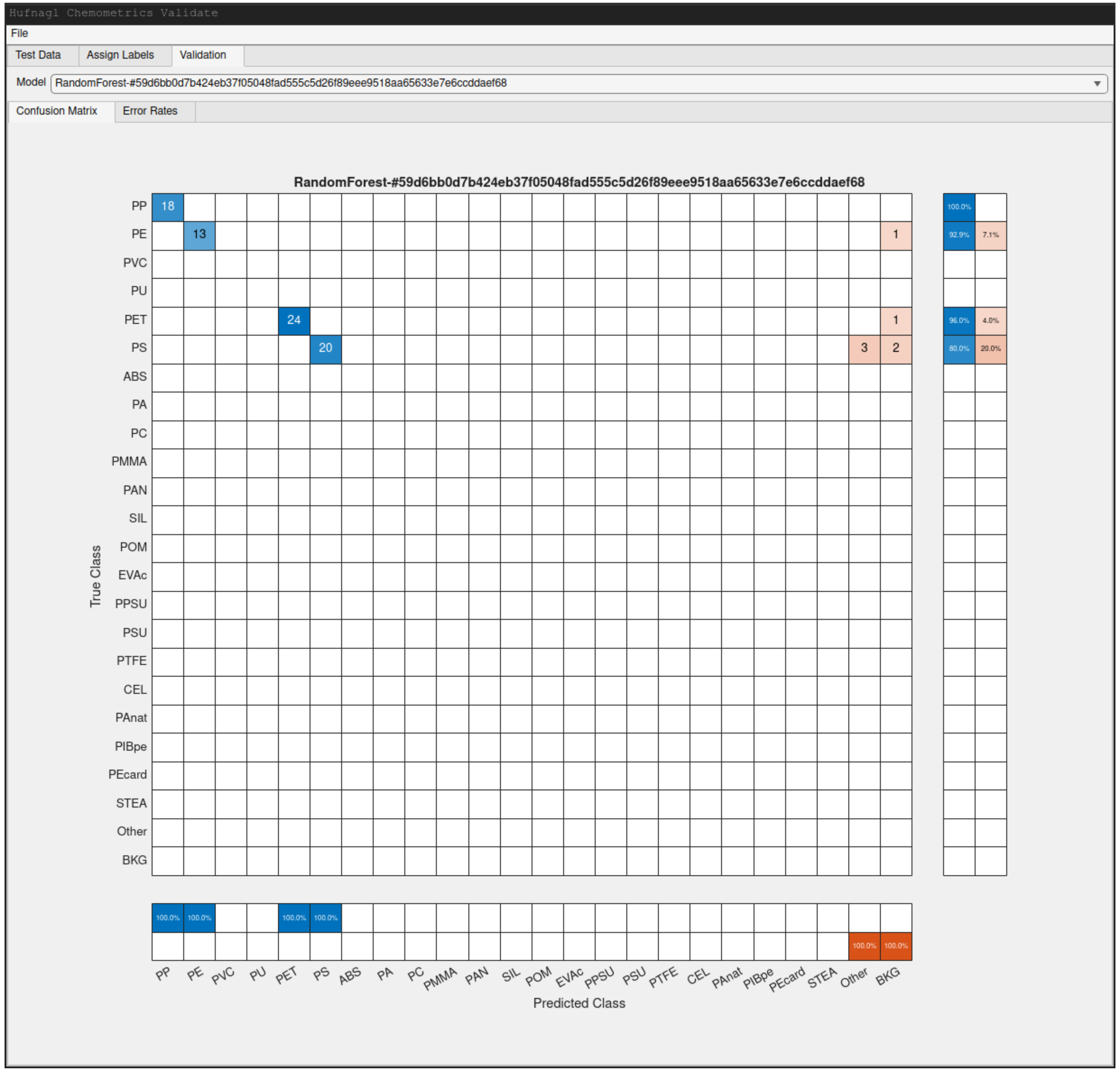

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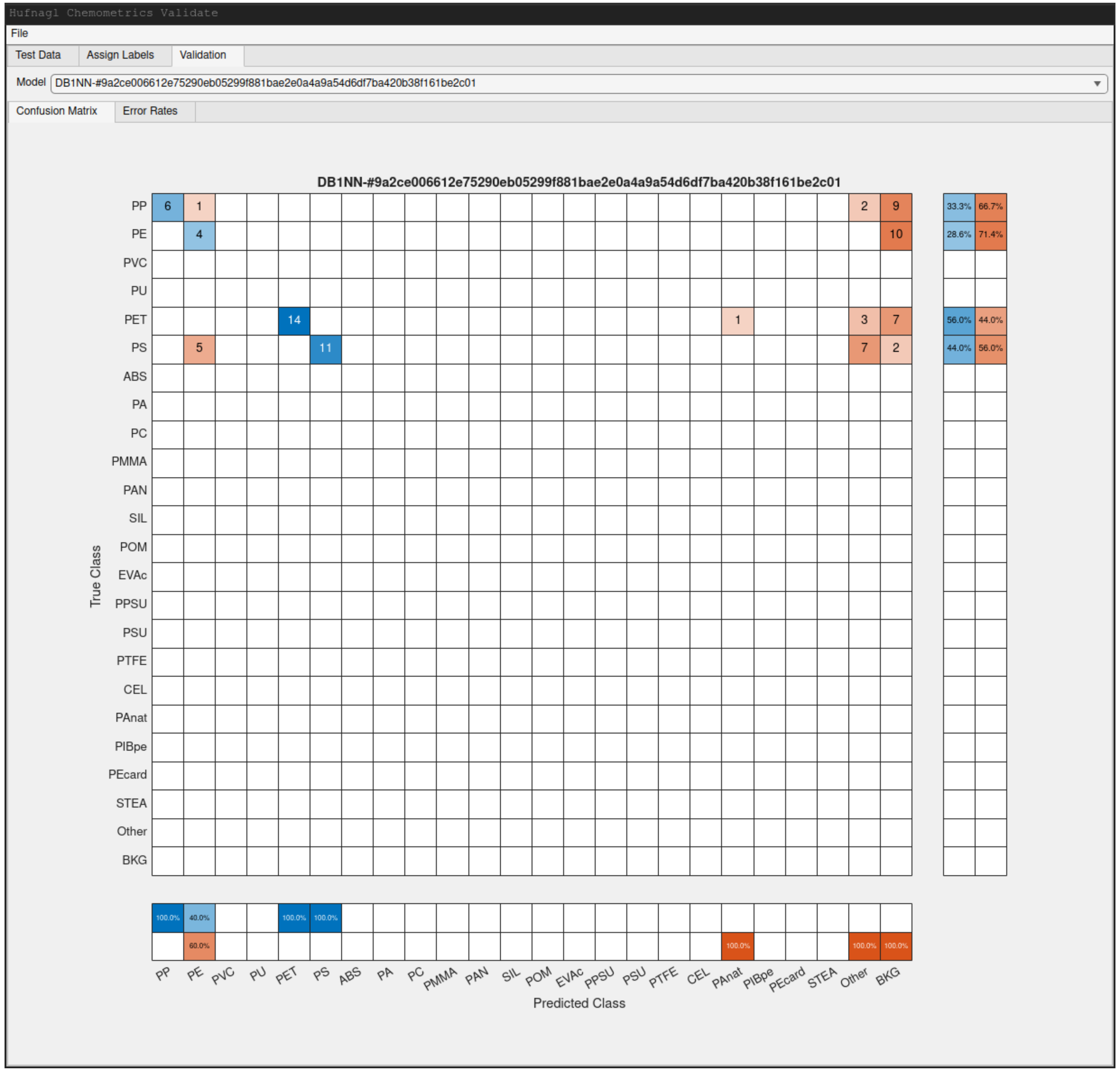

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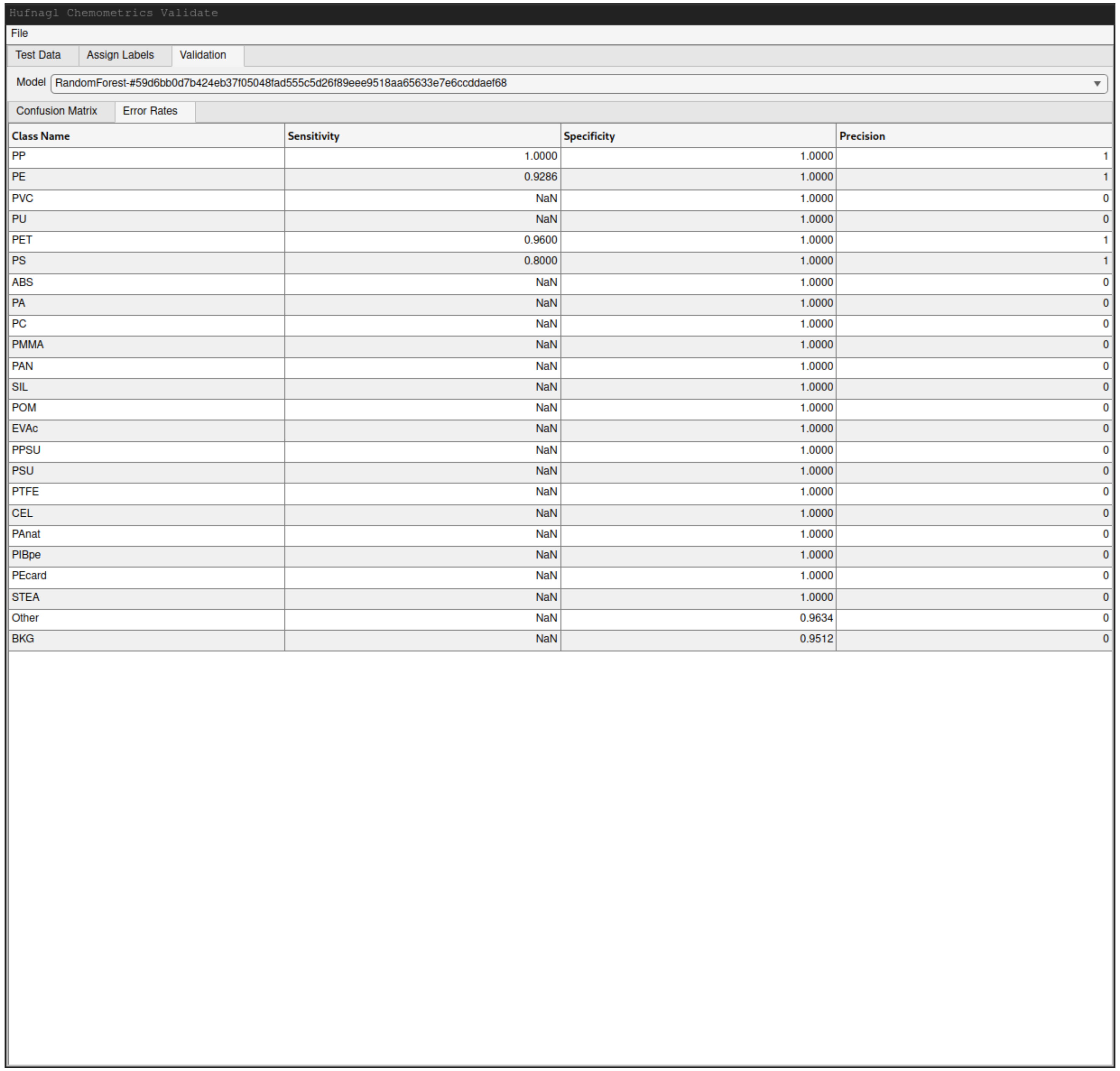

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PU	NaN	1.0000	0
PET	0.9600	1.0000	1
PS	0.8000	1.0000	1
ABS	NaN	1.0000	0
PA	NaN	1.0000	0
PC	NaN	1.0000	0
PMMA	NaN	1.0000	0
PAN	NaN	1.0000	0
SIL	NaN	1.0000	0
POM	NaN	1.0000	0
EVAc	NaN	1.0000	0
PPSU	NaN	1.0000	0
PSU	NaN	1.0000	0
PTFE	NaN	1.0000	0
CEL	NaN	1.0000	0
PAnat	NaN	1.0000	0
PIBpe	NaN	1.0000	0
PEcard	NaN	1.0000	0
STEA	NaN	1.0000	0
Other	NaN	0.9634	0
BKG	NaN	0.9512	0

Dr. Benedikt Hufnagl [a,b]

[a] Austrian Delegate at ISO

[b] Hufnagl Chemometrics GmbH

contact info:
office@hufnagl-chemometrics.com

Hufnagl Chemometrics

Software developments for particle detection and quantification based on FT-IR hyperspectral data

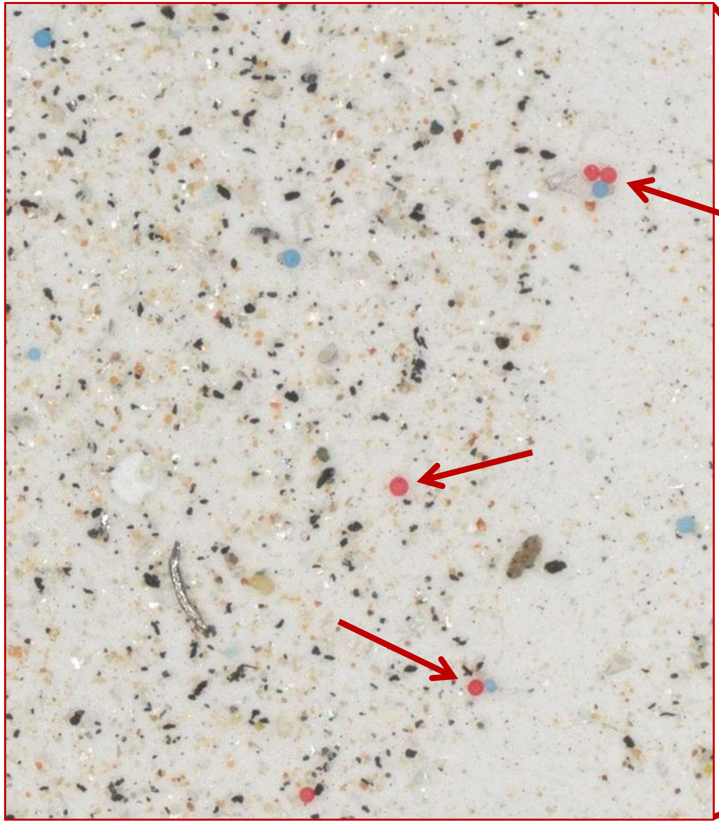
Eric Ceglie, Christoph Hüglin

Empa, Laboratory for Air Pollution and Environmental Technology

Ralf Kägi, Matthias Philipp

Eawag, Process Engineering Department

Surrogates Detection



Problem: We want to count the surrogates

Ultralytics YOLO11 Models

Model	Filenames	Task	Inference	Validation	Training	Export
YOLO11	yolo11n.pt yolo11s.pt yolo11m.pt yolo11l.pt yolo11x.pt	Detection	✅	✅	✅	✅
YOLO11-seg	yolo11n-seg.pt yolo11s-seg.pt yolo11m-seg.pt yolo11l-seg.pt yolo11x-seg.pt	Instance Segmentation	✅	✅	✅	✅
YOLO11-pose	yolo11n-pose.pt yolo11s-pose.pt yolo11m-pose.pt yolo11l-pose.pt yolo11x-pose.pt	Pose/Keypoints	✅	✅	✅	✅
YOLO11-obb	yolo11n-obb.pt yolo11s-obb.pt yolo11m-obb.pt yolo11l-obb.pt yolo11x-obb.pt	Oriented Detection	✅	✅	✅	✅
YOLO11-cls	yolo11n-cls.pt yolo11s-cls.pt yolo11m-cls.pt yolo11l-cls.pt yolo11x-cls.pt	Classification	✅	✅	✅	✅

Currently, we are only using these two.

- YOLO11 is collection of a cutting-edge **pre-trained AI models** for **computer vision tasks**.
- It includes models for detection, segmentation, classification, and more.
- Designed for efficiency, it achieves **high accuracy with small training data sets**.
- Versatile and scalable for research and real-world applications.

How is it Licensed?

Ultralytics offers two licensing options for YOLO:

- **AGPL-3.0 License:** This open-source license is ideal for educational and non-commercial use, promoting open collaboration.
- **Enterprise License:** This is designed for commercial applications, allowing seamless integration of Ultralytics software into commercial products without the restrictions of the AGPL-3.0 license.

"Our licensing strategy is designed to ensure that any improvements to our open-source projects are returned to the community. We hold the principles of open source close to our hearts 💗, and our mission is to guarantee that our contributions can be utilized and expanded upon in ways that are beneficial to all."

[Source: https://docs.ultralytics.com/#yolo-a-brief-history]

BibTeX

```
@software{yolo11_ultralytics,
  author = {Glenn Jocher and Jing Qiu},
  title = {Ultralytics YOLO11},
  version = {11.0.0},
  year = {2024},
  url = {https://github.com/ultralytics/ultralytics},
  orcid = {0000-0001-5950-6979, 0000-0002-7603-6750, 0000-0003-3783-7069},
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}
```
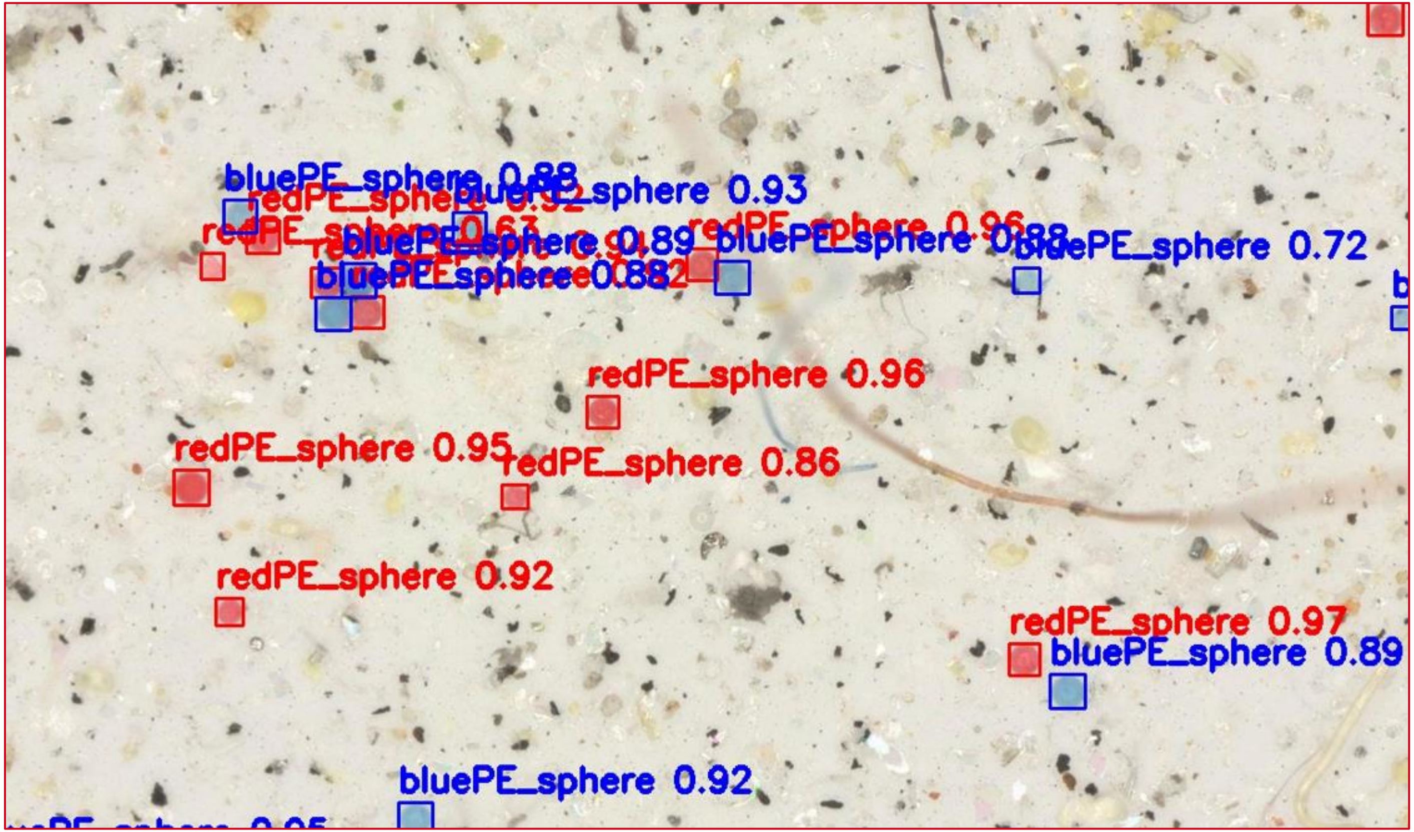
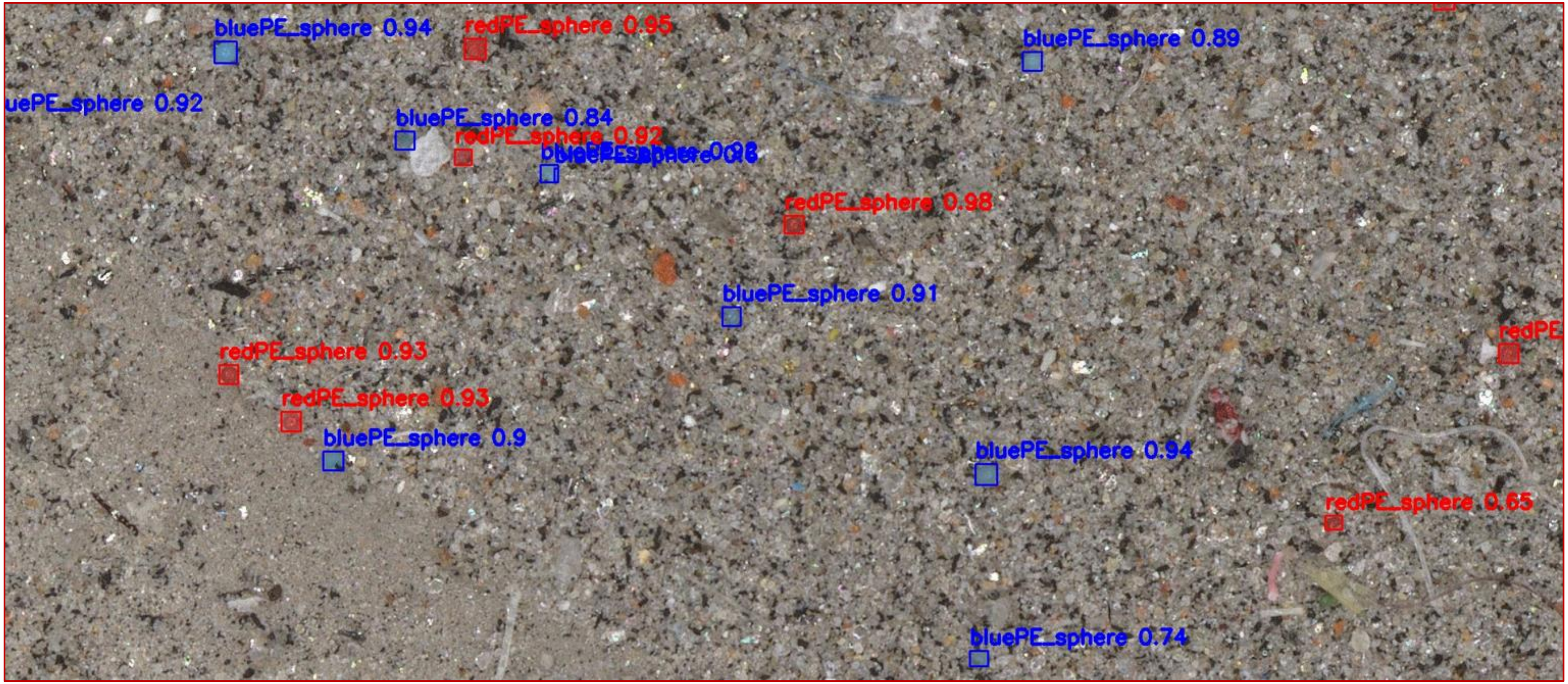
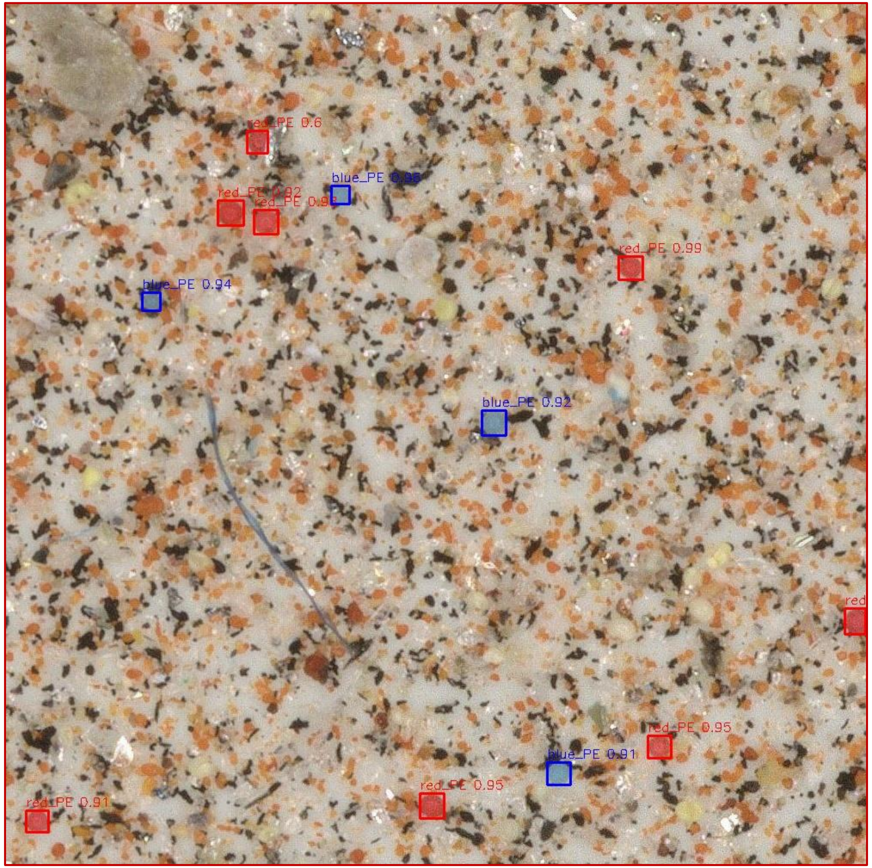

Surrogates Detection: Results



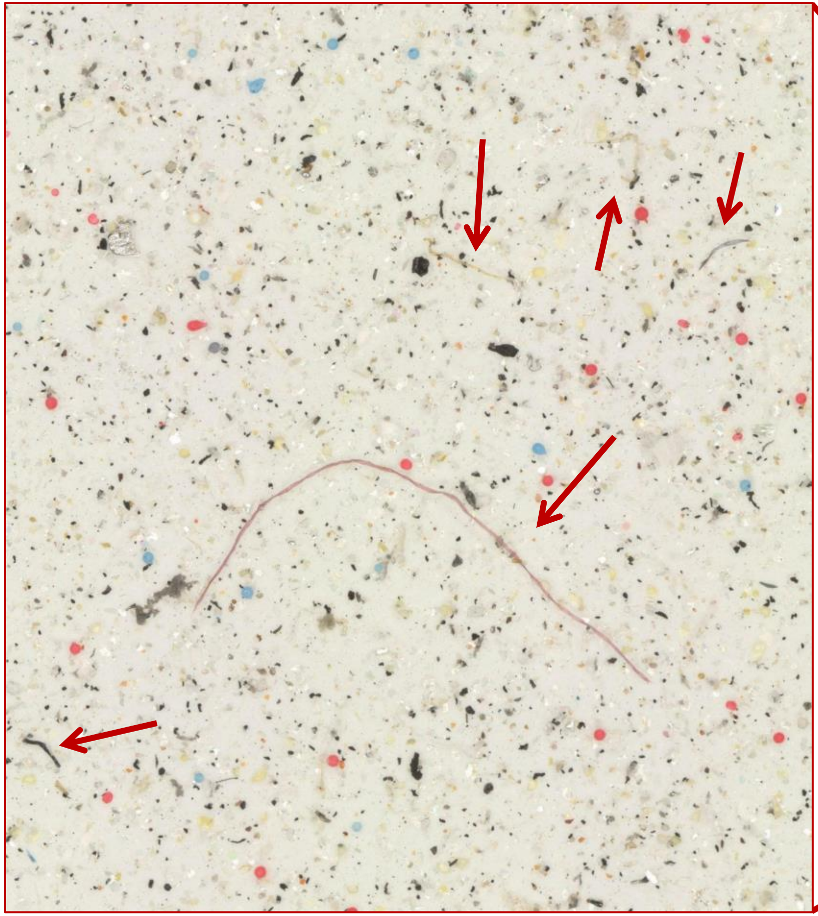
Surrogates Detection: Results



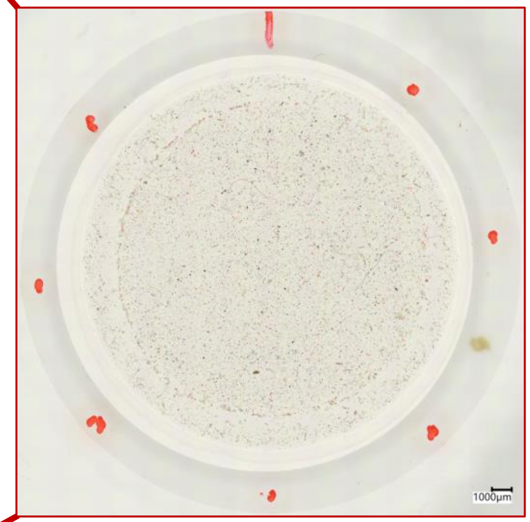
Surrogates Detection: Results



Fiber Detection: Results

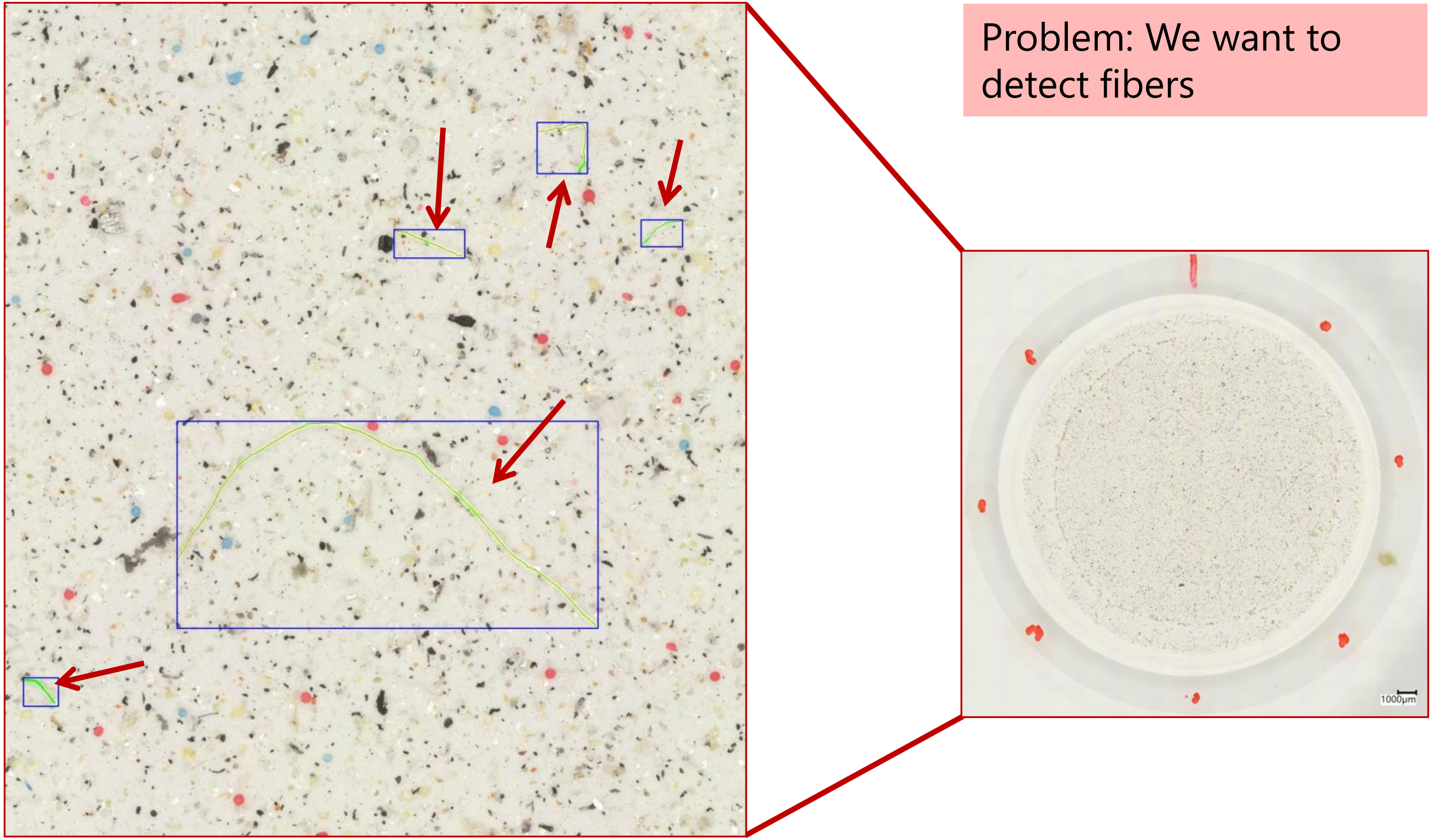


Problem: We want to detect fibers

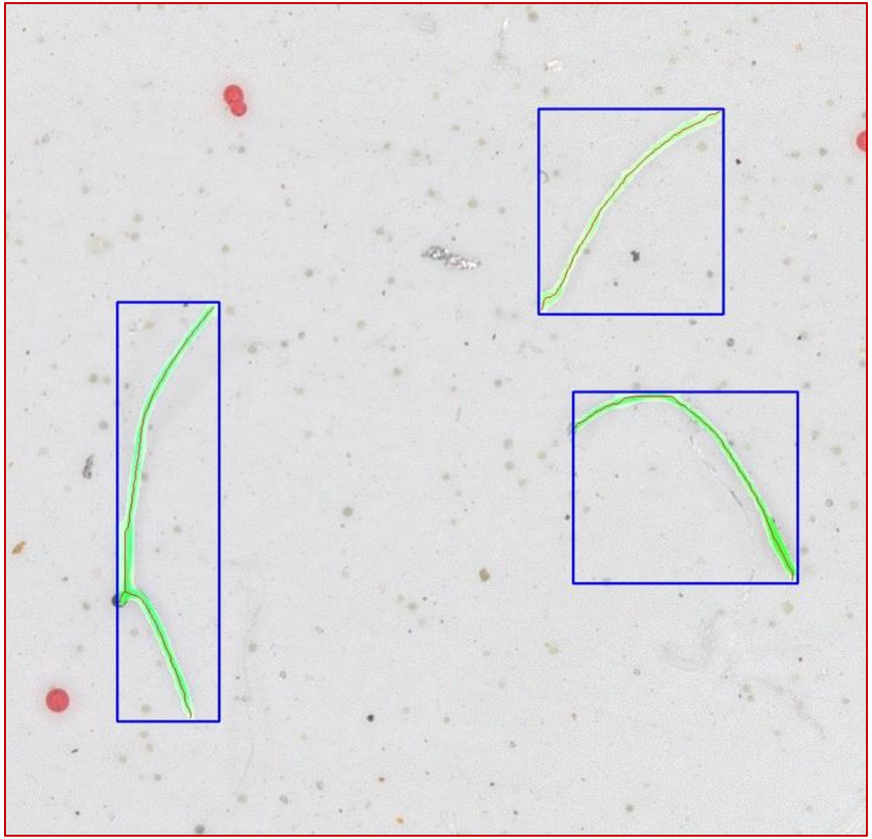


Fiber Detection: Results

Problem: We want to detect fibers

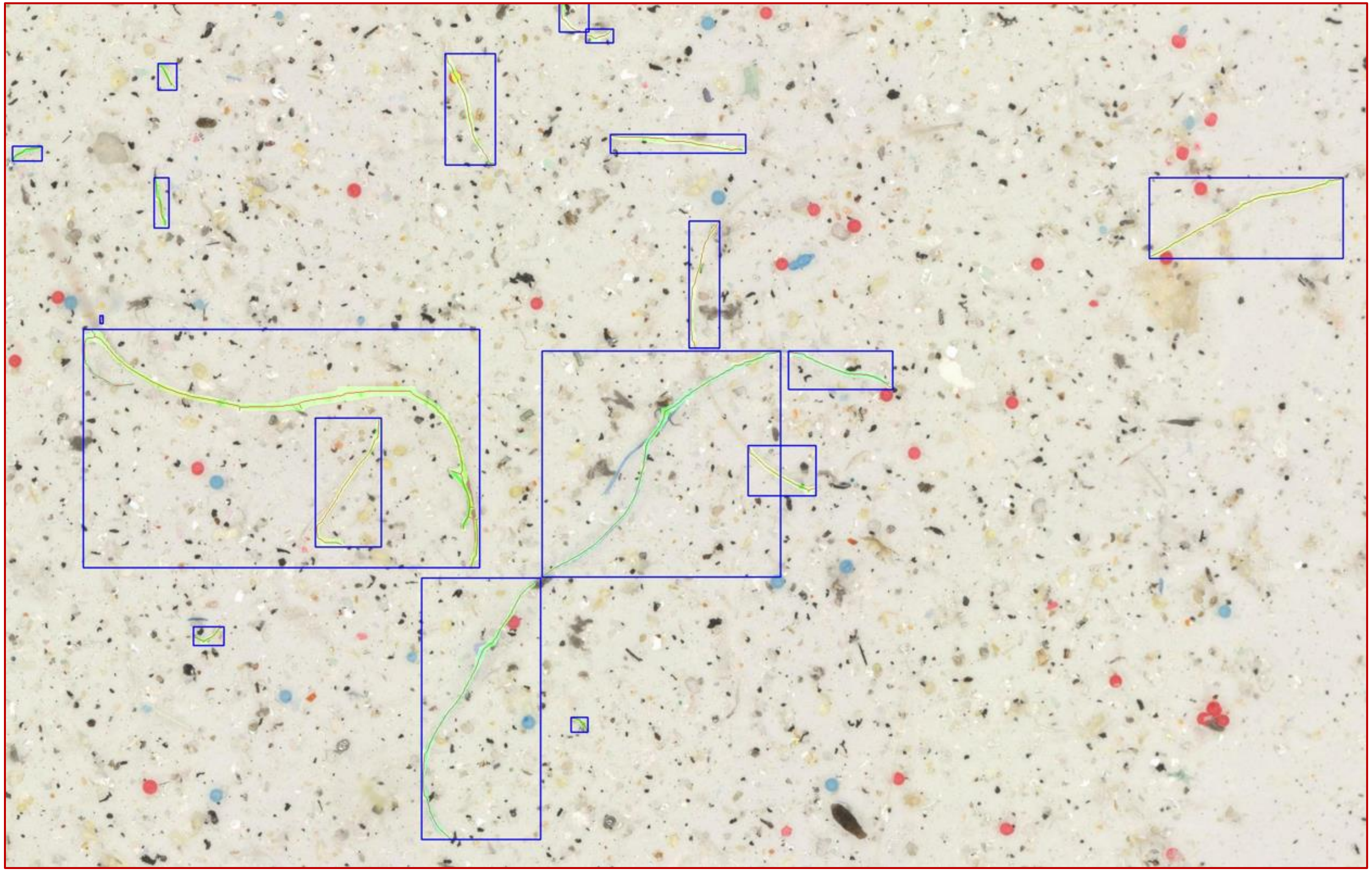


Fiber Detection: Results

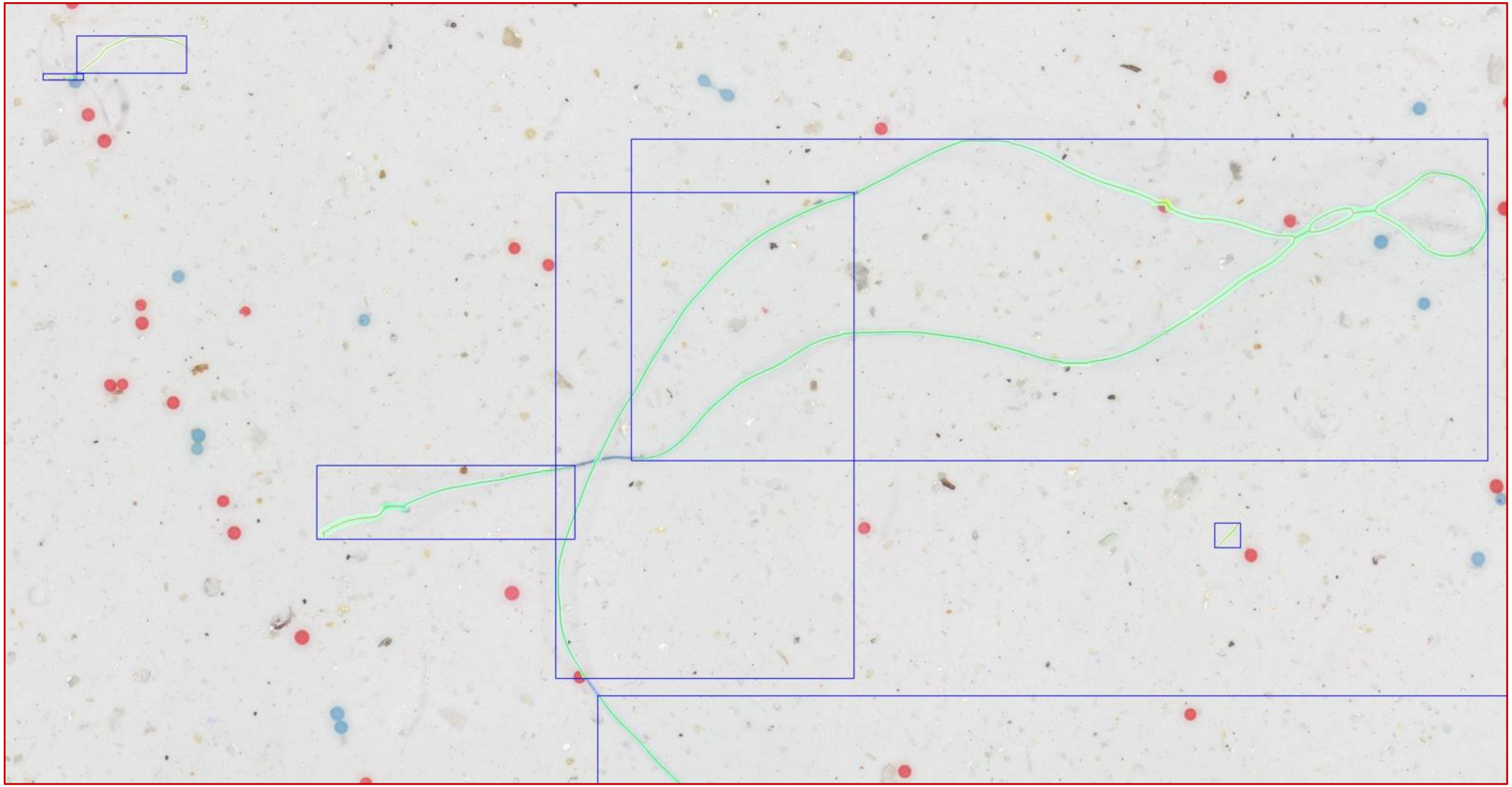


Fiber Detection: Results

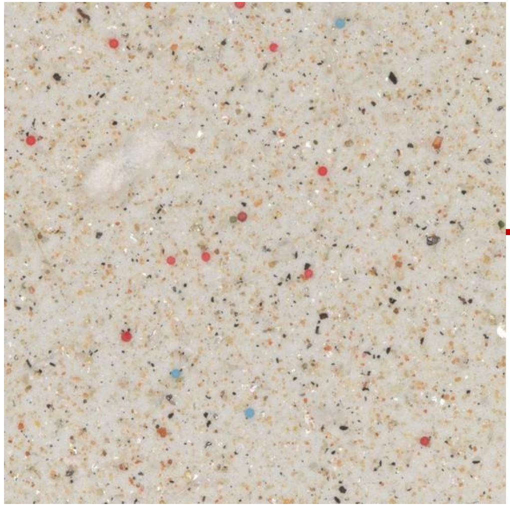
Fiber Detection: Results



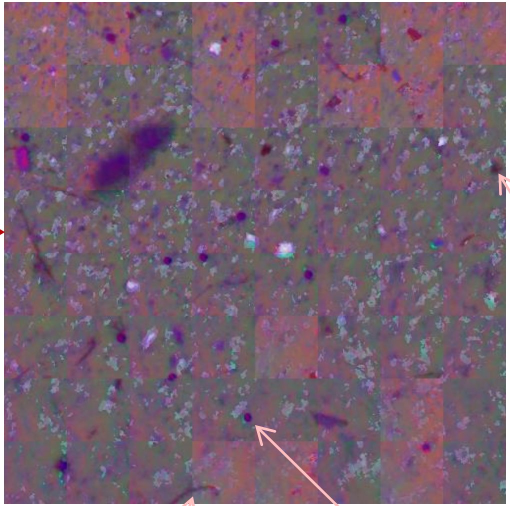
Fiber Detection: Results



Spectral Classification

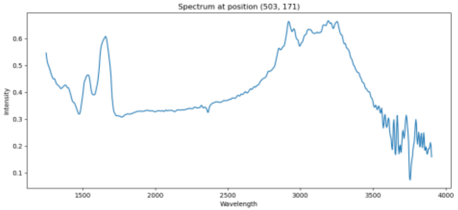


FTIR spectroscopy

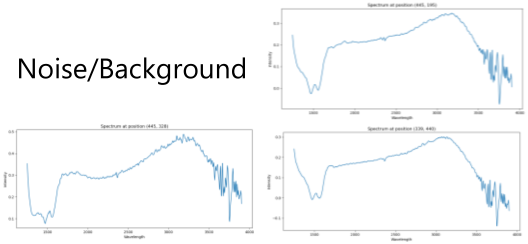


Problem: Classify Spectral Data of microplastics samples

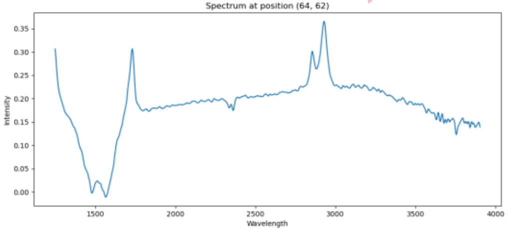
Polyamide (?)



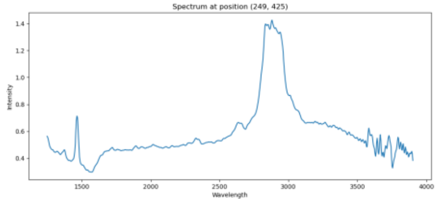
Noise/Background



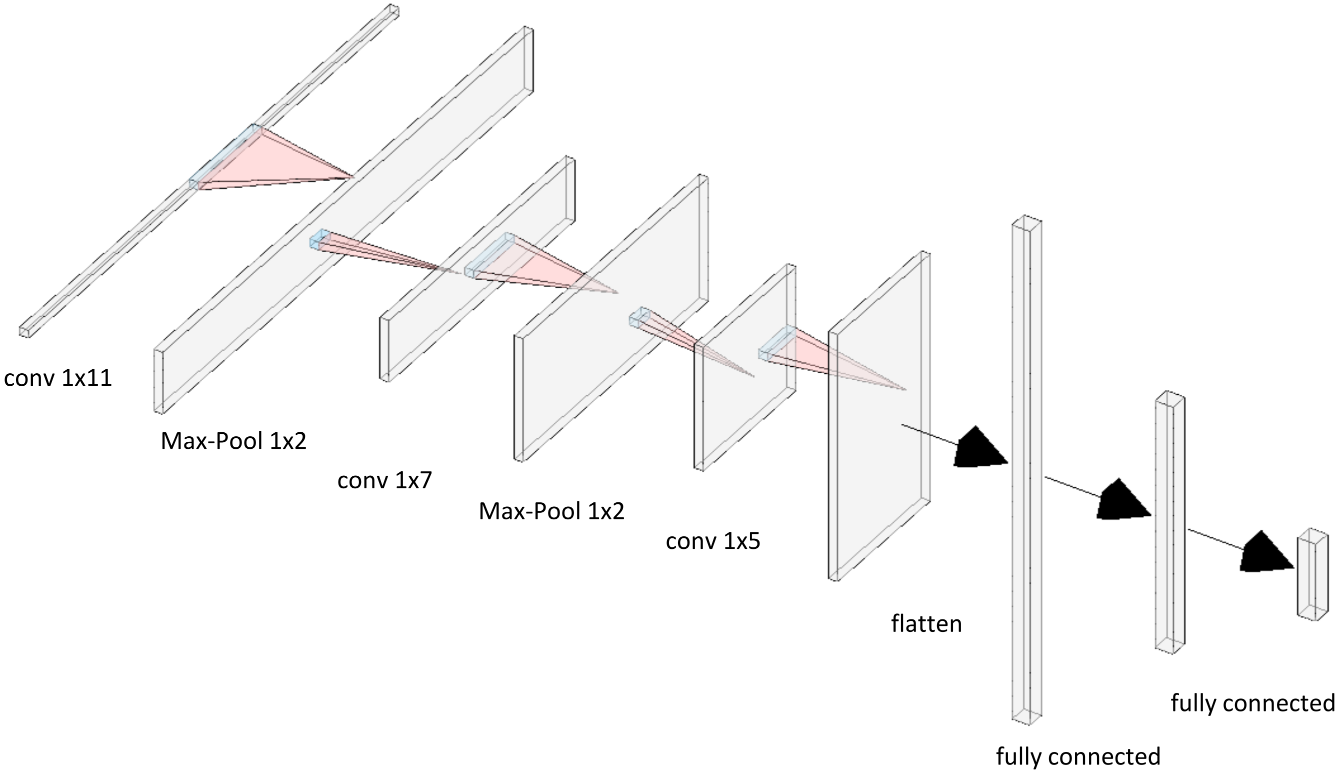
PET (?)



Polyethylene



Spectral Classification: Model Architecture (CNN)



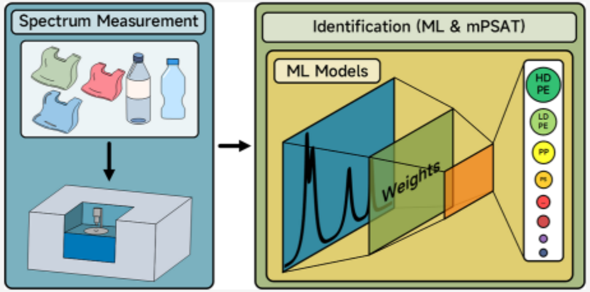
Why should we use a CNN?

Spectral Classification of Large-Scale Blended (Micro)Plastics Using FT-IR Raw Spectra and Image-Based Machine Learning

Yanlong Liu, Wenli Yao, Fenghui Qin, Lei Zhou,* and Yian Zheng*

Cite This: *Environ. Sci. Technol.* 2023, 57, 6656–6663

ABSTRACT: Microplastics (MPs) are currently recognized as emerging pollutants; their identification and classification are therefore essential during their monitoring and management. In contrast to most studies based on small datasets and library searches, this study developed and compared four machine learning-based classifiers and two large-scale blended plastic datasets, where a 1D convolutional neural network (CNN), decision tree, and random forest (RF) were fed with raw spectral data from Fourier transform infrared spectroscopy, while a 2D CNN used the corresponding spectral images as the input. With an overall accuracy of 96.43% on a small dataset and 97.44% on a large dataset, the 1D CNN outperformed other models. The 1D CNN was the best at predicting environment samples, while the RF was the most robust with less spectral data. Overall, RF and 2D CNNs might be evaluated for plastic identification with fewer spectral data; however, 1D CNNs were thought to be the most effective with sufficient spectral data. Accordingly, an open-source MP spectroscopic analysis tool was developed to facilitate a quick and accurate analysis of existing MP samples.



KEYWORDS: *microplastic, classification, FT-IR, neural network, machine learning*

Why should we use a CNN?

Results from Liu, Yanlong, et al. "Spectral classification of large-scale blended (Micro) plastics using FT-IR raw spectra and image-based machine learning." *Environmental Science & Technology* 57.16 (2023): 6656-6663.

Purency uses this (see [1], [2])

We use this

Table 1. Overall Accuracy, Recall, Precision, and F_1 of DT, RF, CNN1D, and CNN2D Trained with DS300[a]

model	accuracy (%)	precision (%)	recall (%)	F_1 (%)
DT	79.22(0.07)	79.73(0.08)	79.13(0.07)	79.20(0.07)
RF	90.59(0.13)	91.02(0.14)	90.62(0.13)	90.60(0.13)
CNN1D	96.43(0.13)	96.64(0.14)	96.44(0.14)	96.47(0.14)
CNN2D	93.87(0.13)	94.02(0.13)	93.87(0.13)	93.88(0.13)

[a]The numbers in brackets represent the standard deviation.

Table 2. Overall Accuracy, Precision, Recall, and F_1-Score of DT, RF, CNN1D, and CNN2D Trained with DS1000[a]

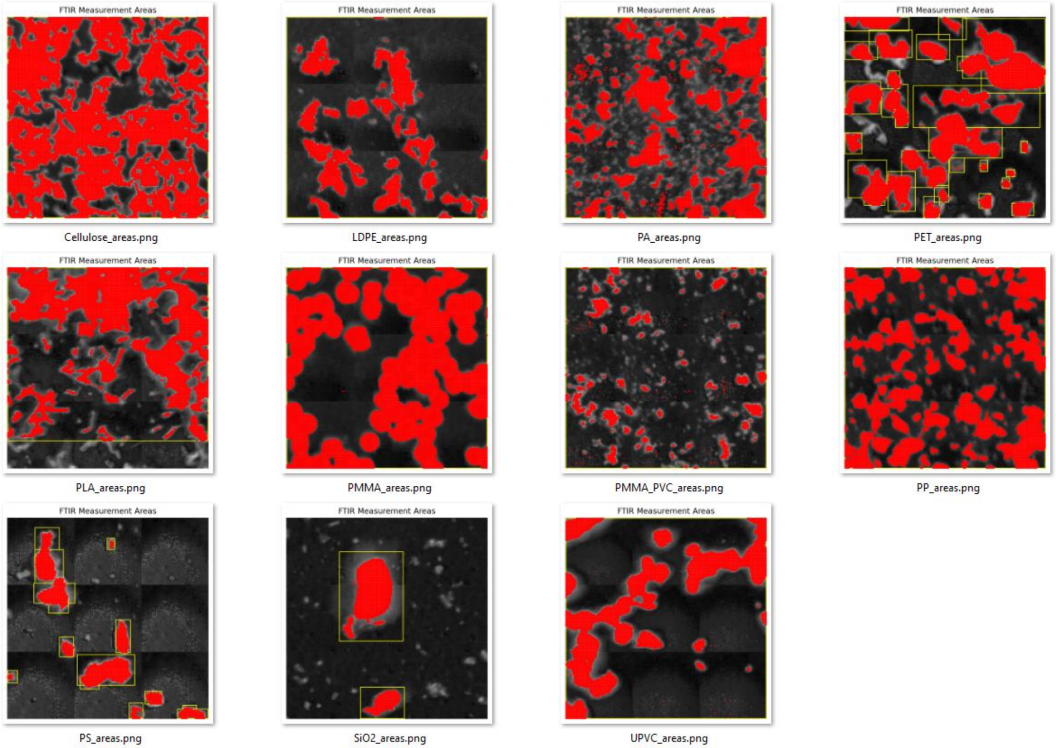
model	accuracy (%)	precision (%)	recall (%)	F_1 (%)
DT	83.14(0.04)	82.68(0.04)	82.86(0.04)	82.66(0.04)
RF	92.59(0.07)	92.55(0.08)	92.42(0.08)	92.36(0.08)
CNN1D	97.44(0.12)	97.55(0.10)	97.38(0.13)	97.42(0.12)
CNN2D	94.89(0.05)	94.90(0.06)	94.81(0.05)	94.81(0.05)

[a]The numbers in brackets represent the standard deviation.

[1] Hufnagl, Benedikt, et al. "A methodology for the fast identification and monitoring of microplastics in environmental samples using random decision forest classifiers." *Analytical Methods* 11.17 (2019): 2277-2285.

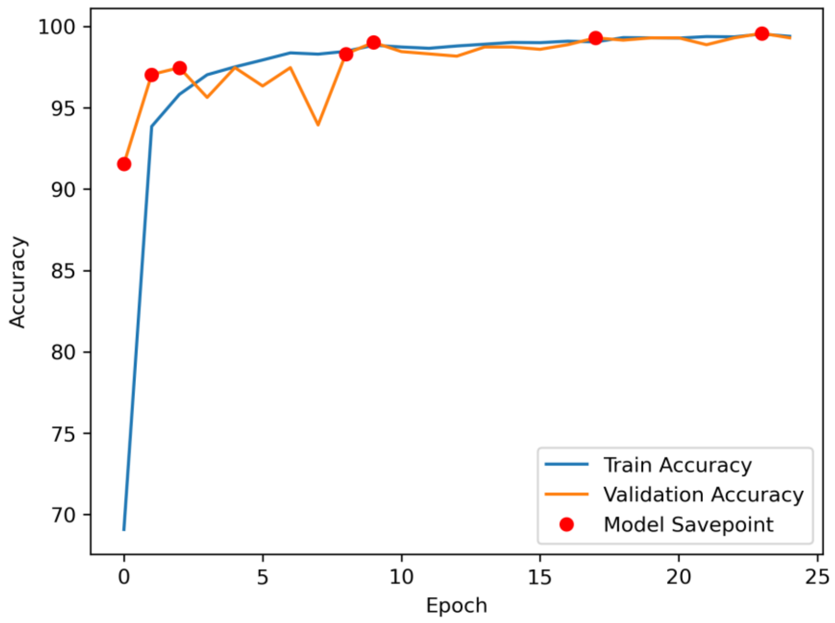
[2] Hufnagl, Benedikt, et al. "Computer-assisted analysis of microplastics in environmental samples based on μFTIR imaging in combination with machine learning." *Environmental science & technology letters* 9.1 (2021): 90-95.

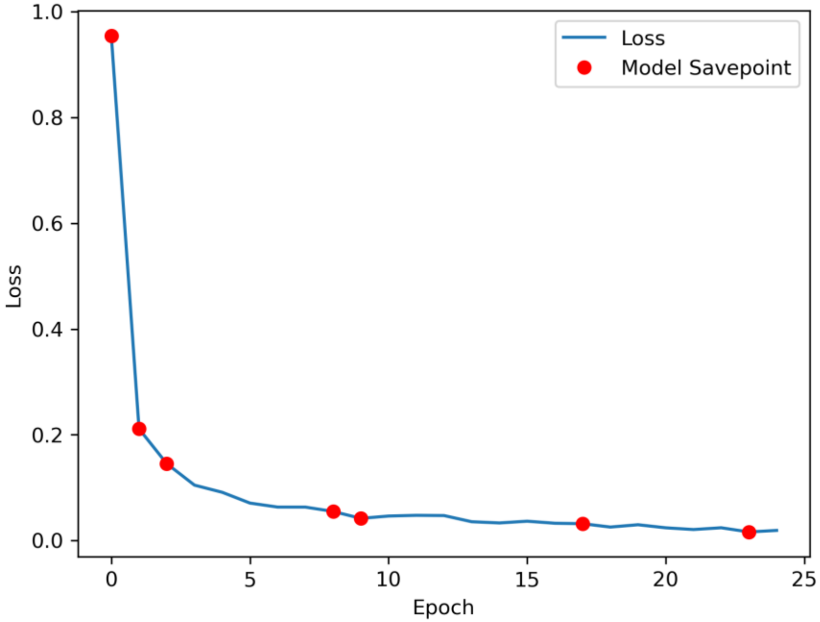
Spectral Classification: Building a Dataset (Reference Data)



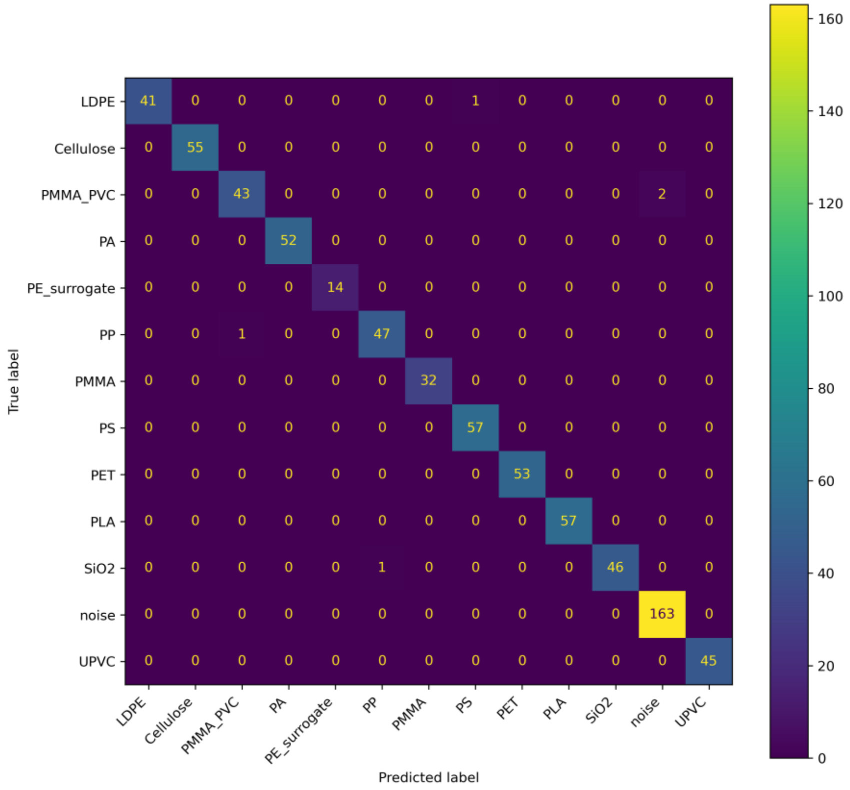
- Each square shows a different material scanned with FT-IR spectroscopy (Agilent).
- Red areas are manually labeled for material (vs. background).
- Dataset includes common plastics (PE, PP, PS, etc.).
- Measurements by Matthias Philipp (Eawag).
- Used to train models for spectral classification.
- Hope: Building our own Dataset the training data is closer to real-world data.

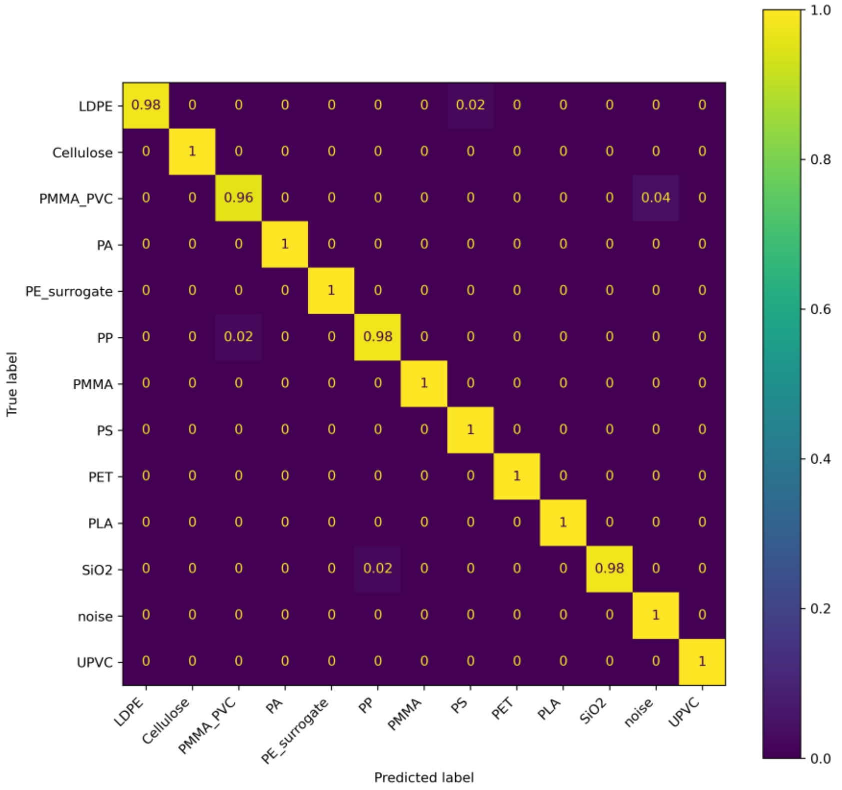
Spectral Classification: Training



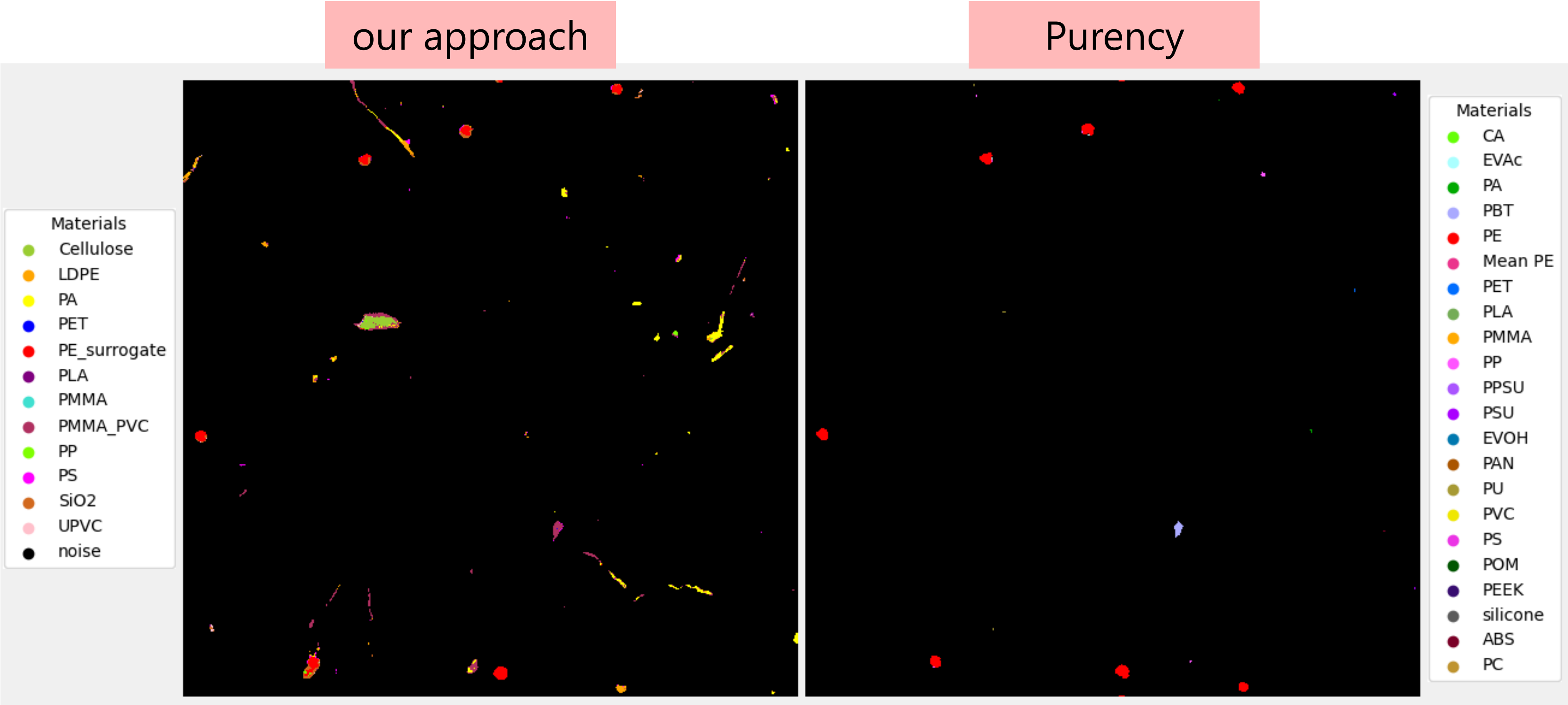


Spectral Classification: Confusion Matrix

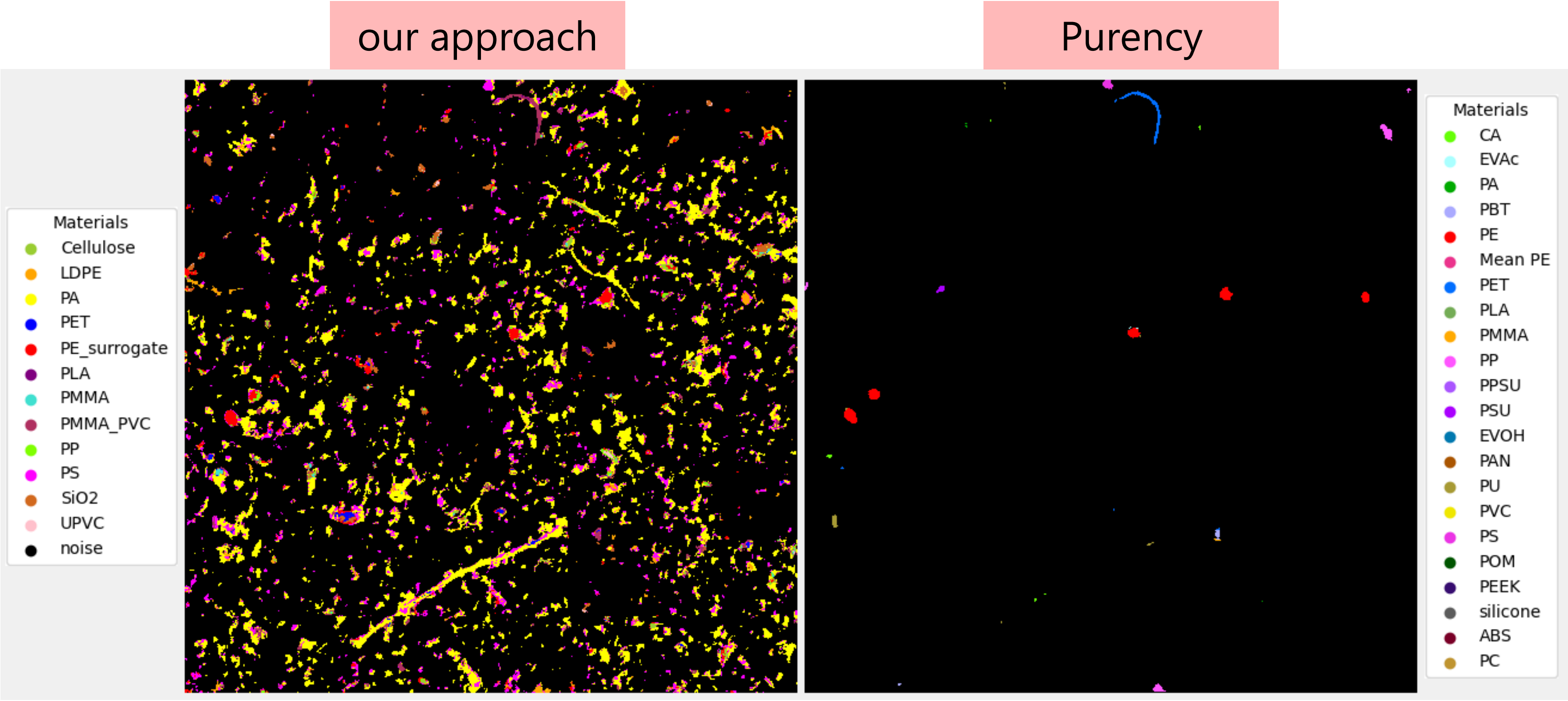




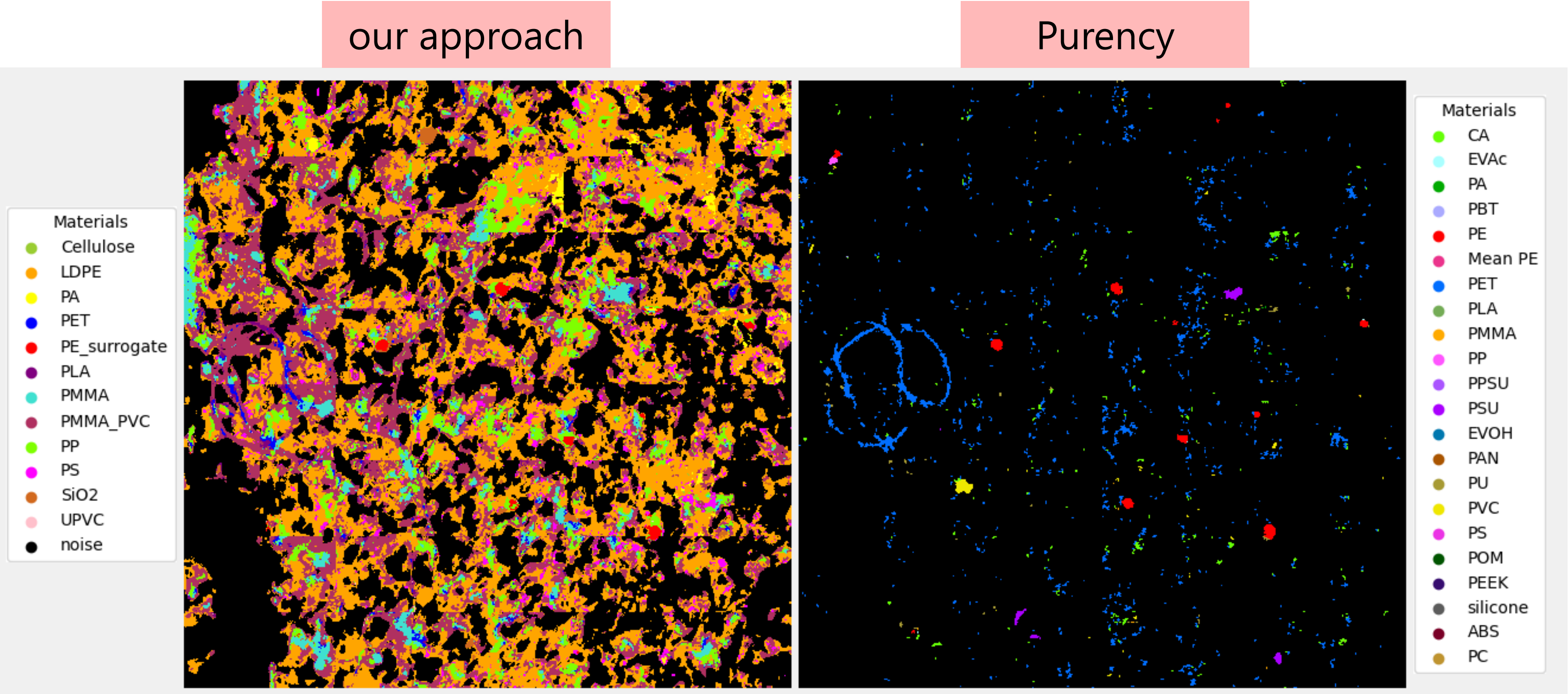
Spectral Classification: First Results



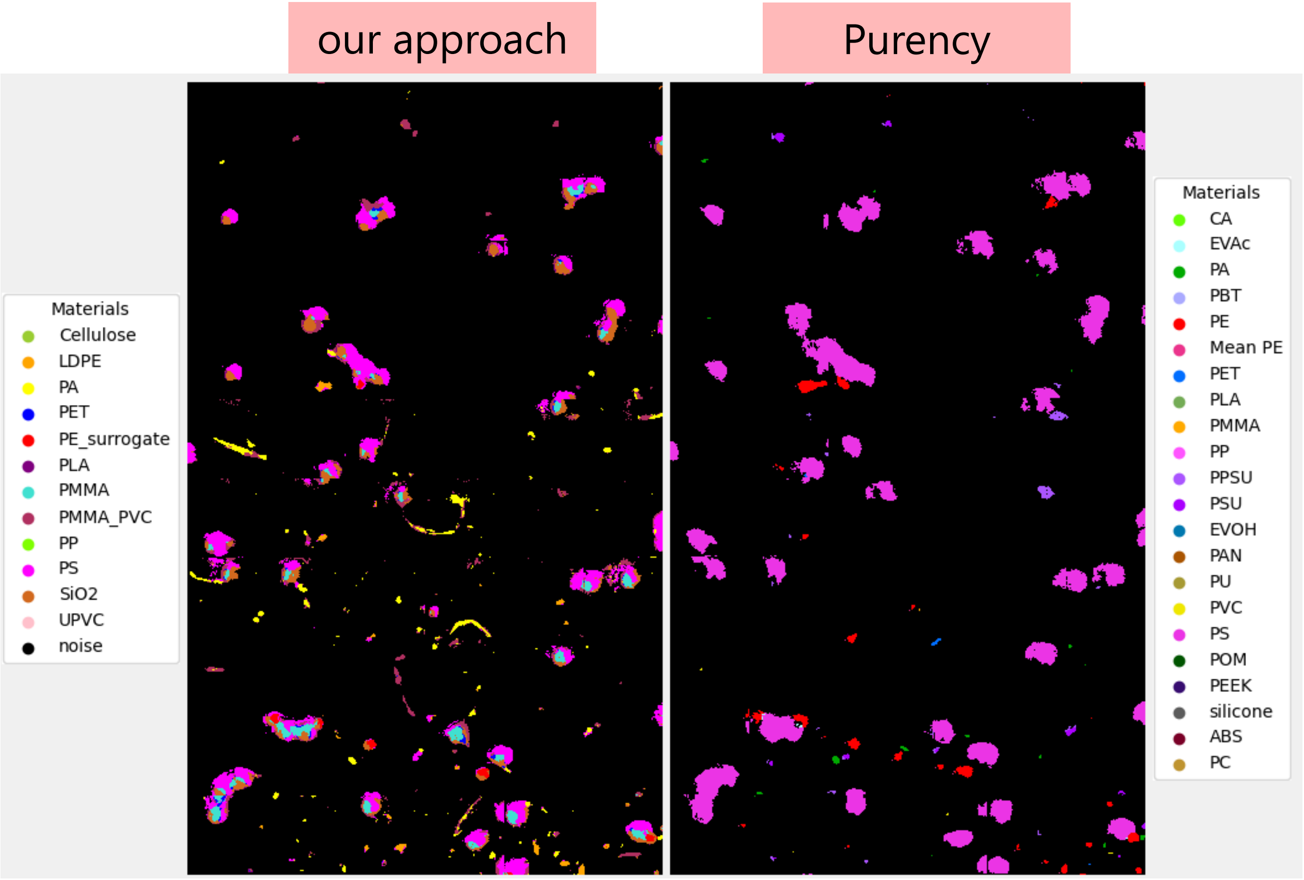
Spectral Classification: First Results



Spectral Classification: First Results

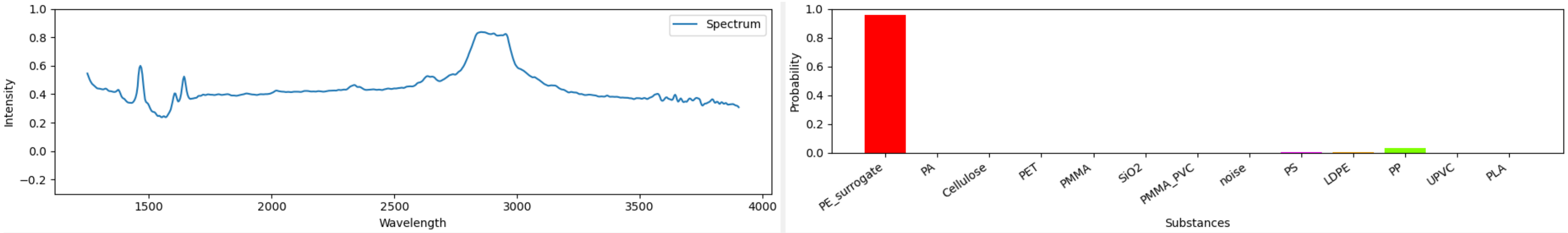


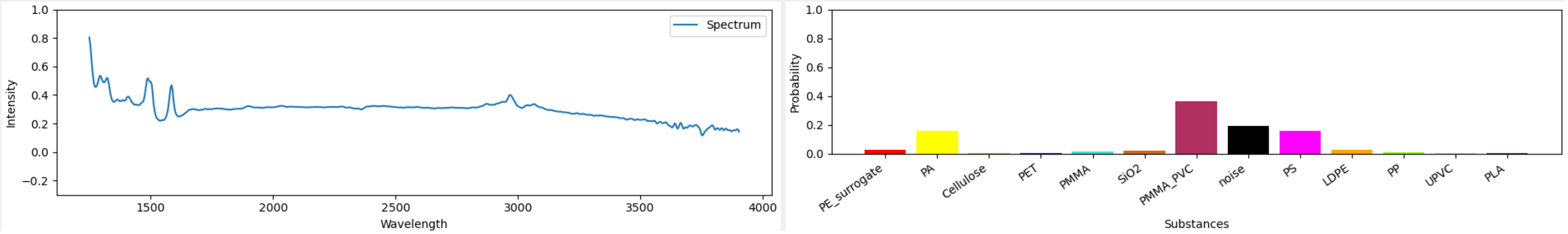
Spectral Classification: First Results



Spectral Classification: First Results

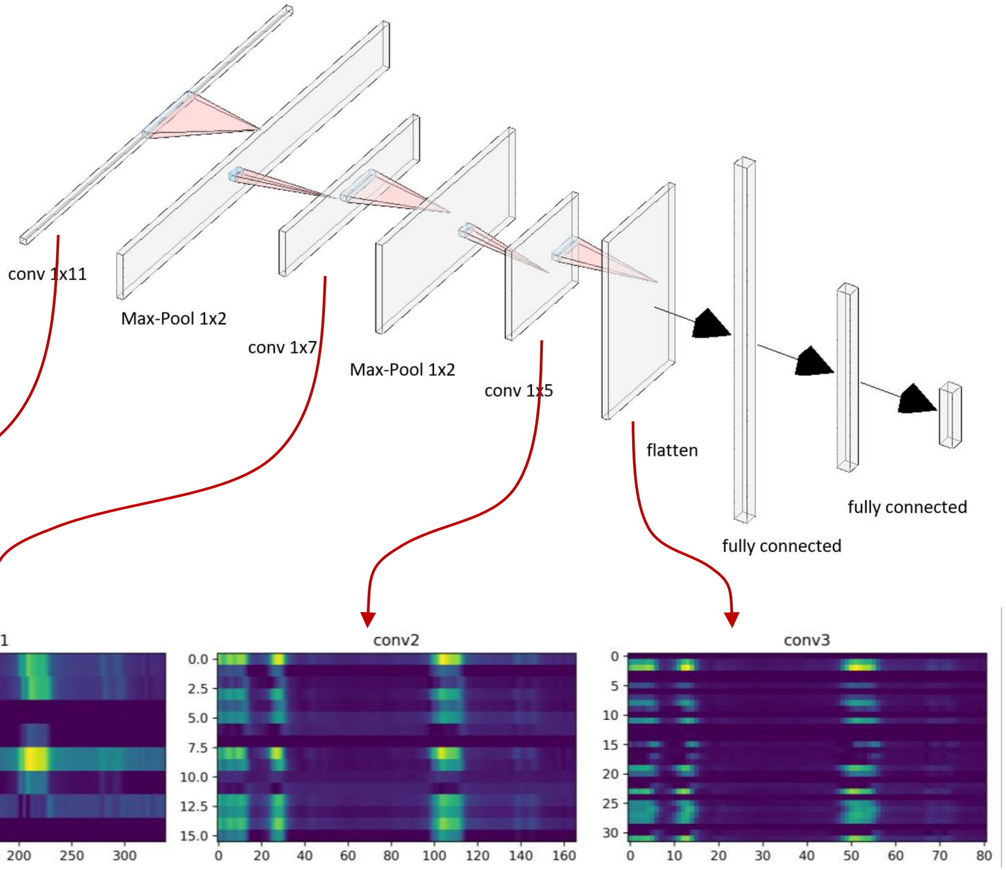
Probability distribution
for classifications





Spectral Classification: Interpretability

- **Goal**: Understand how the model learns spectral features for material classification.
- **Architecture**: A 1D CNN processes input spectra through convolution layers.
- **Feature Maps**: Visualized at different convolutional layers (conv1–conv3) to visualize learned patterns.
- **Interpretability**: Helps identify which parts of the spectrum are important for classification decisions.



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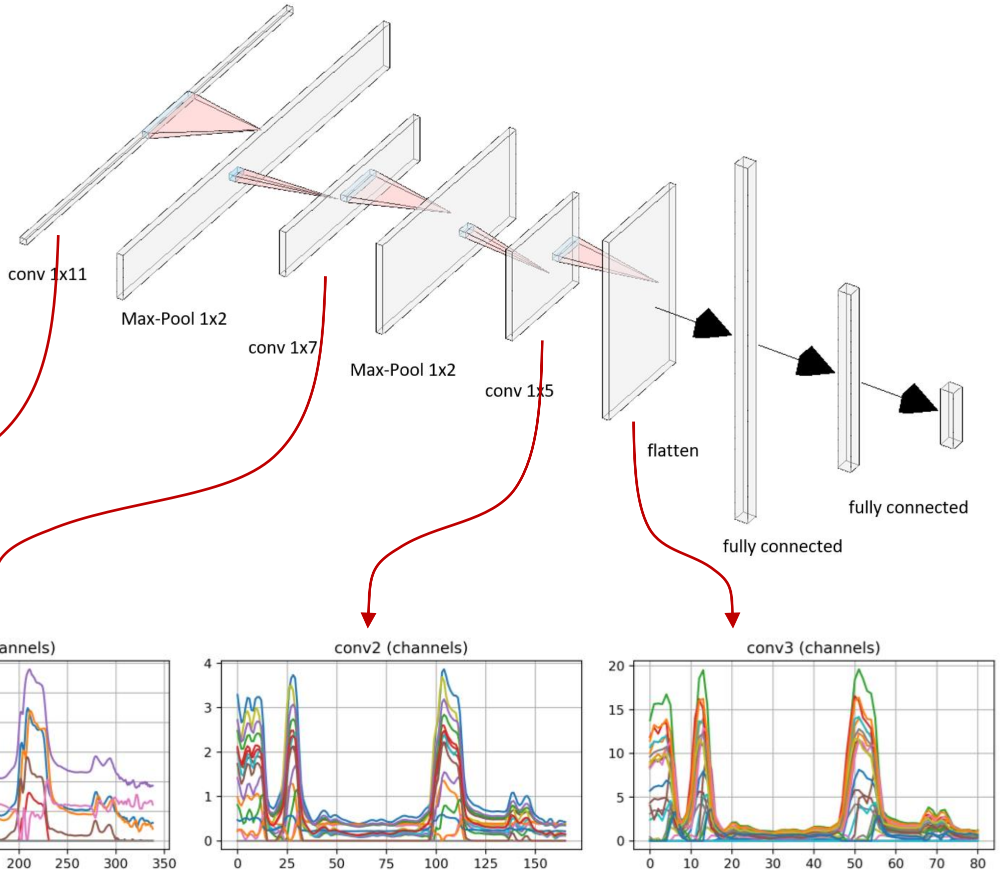
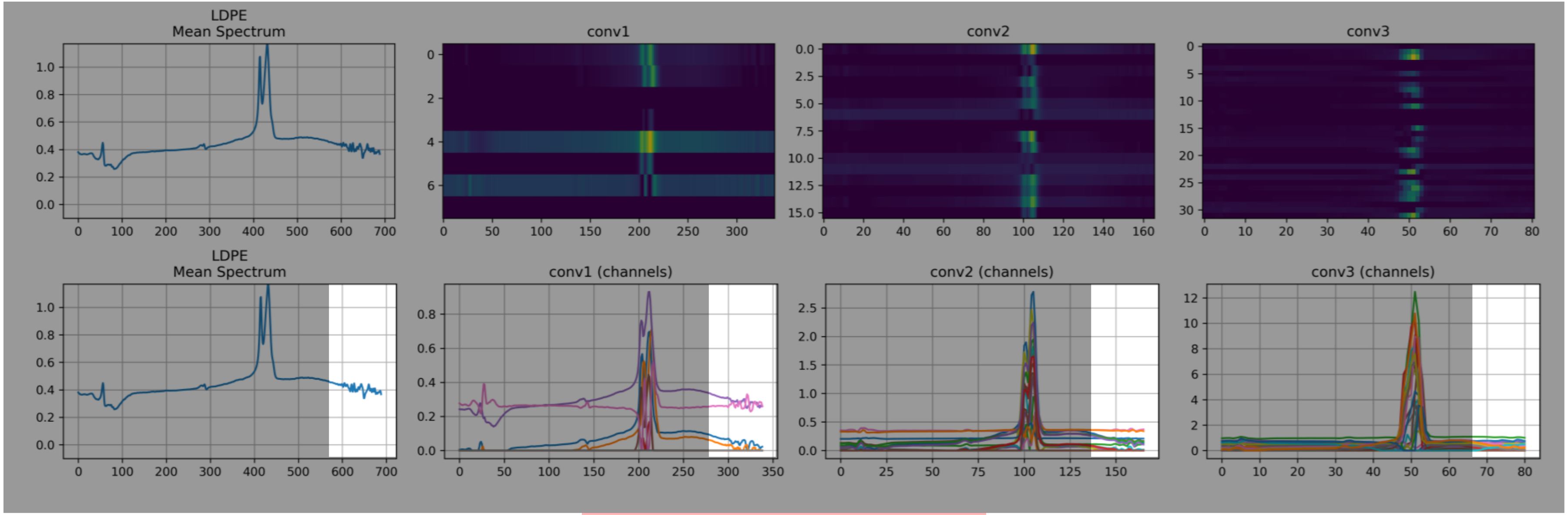


Spectral Classification: Interpretability

Example: LDPE

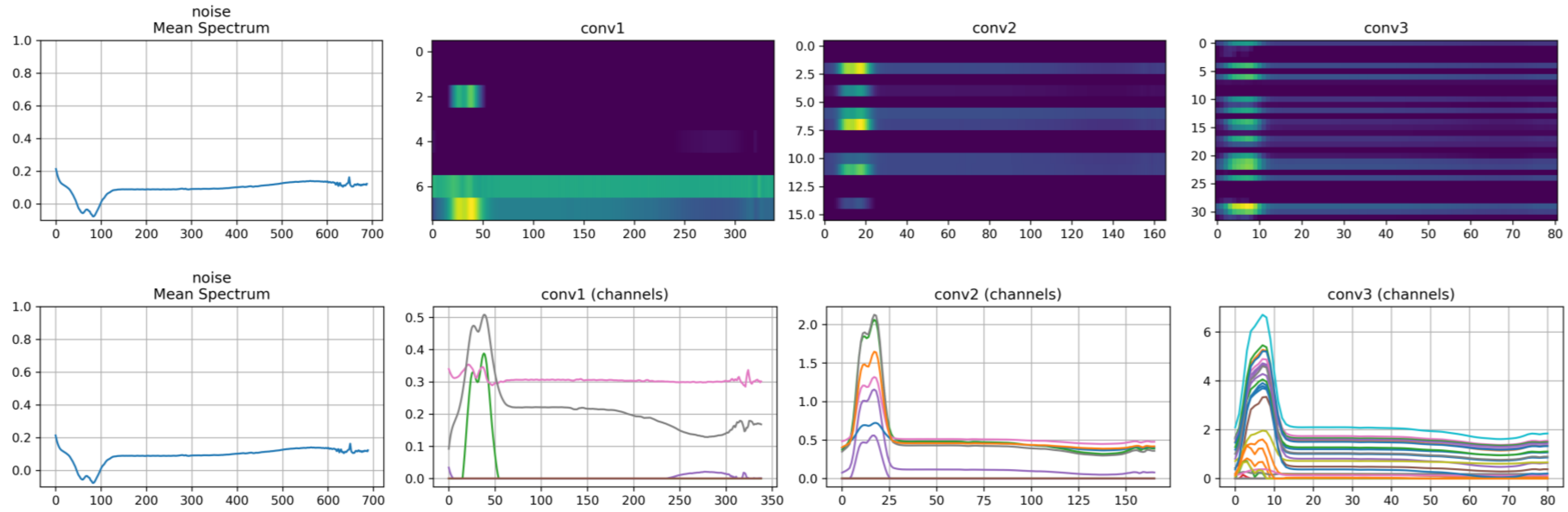


Observation: Pattern fades away in deeper convolutional layers

→ **Interpretation:** This pattern is likely not relevant for the classification

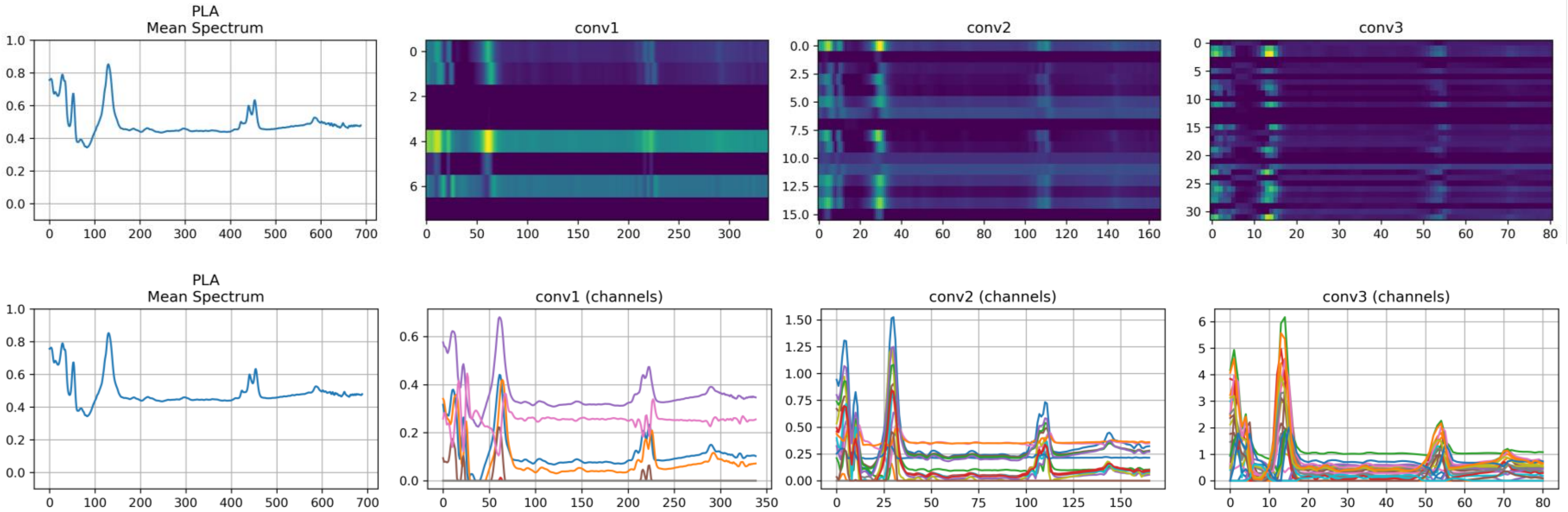
Spectral Classification: Interpretability

Example: Noise



Spectral Classification: Interpretability

Example: PLA



Next Steps

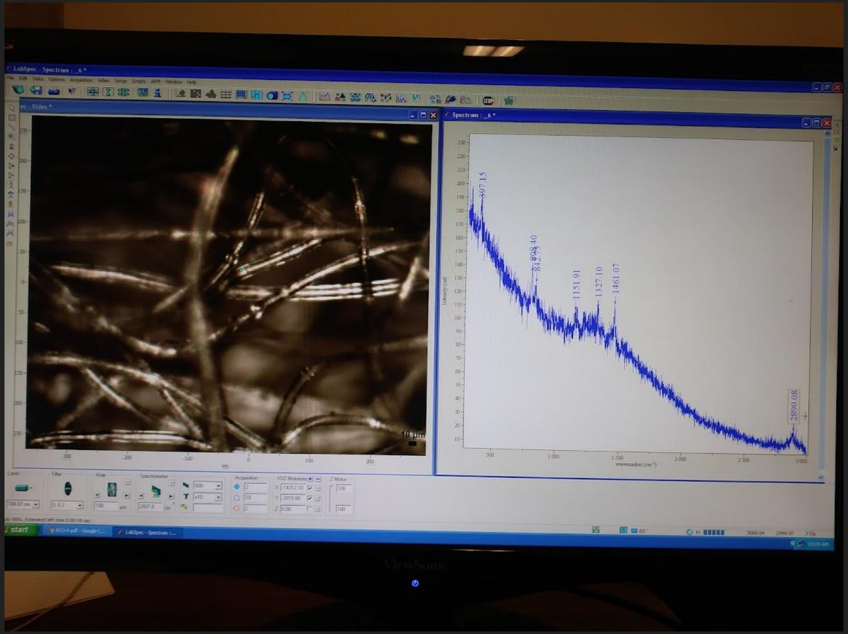
- Improve/extend reference data set (better separation from background, include more samples)
- Improve model architecture based on feature maps
- Include spectral matching in Yamanaka software
- Write stand-alone software to easily run spectral matching

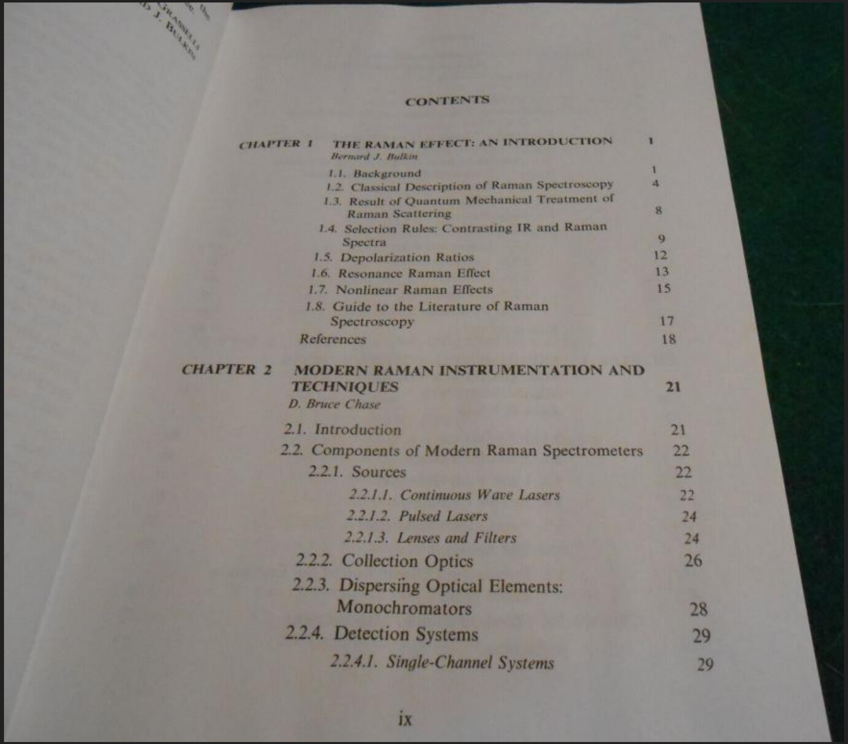
Acknowledgements: Thanks to the Swiss Federal Office for the Environments (FOEN) for funding projects at Empa and Eawag on environmental microplastics.

Automated microplastic spectroscopy, biases, limitations, and opportunities

Dr. Win Cowger
Research Director
Moore Institute for Plastic Pollution Research

When I started microplastic spectral analysis

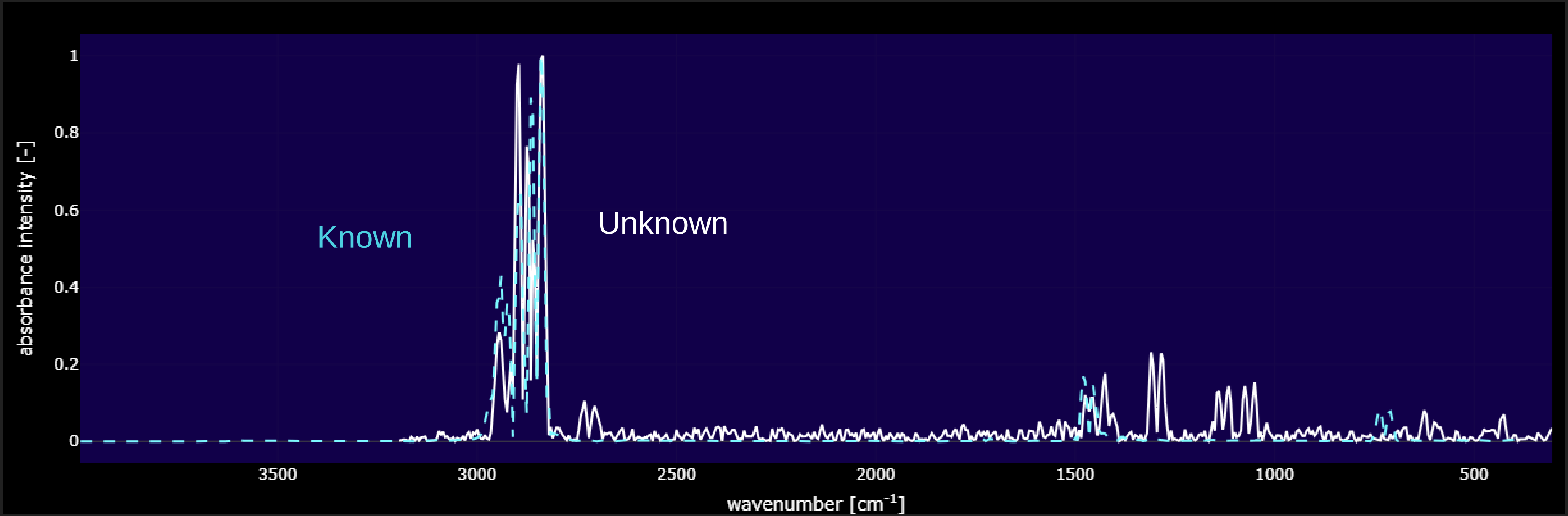




CONTENTS

ix

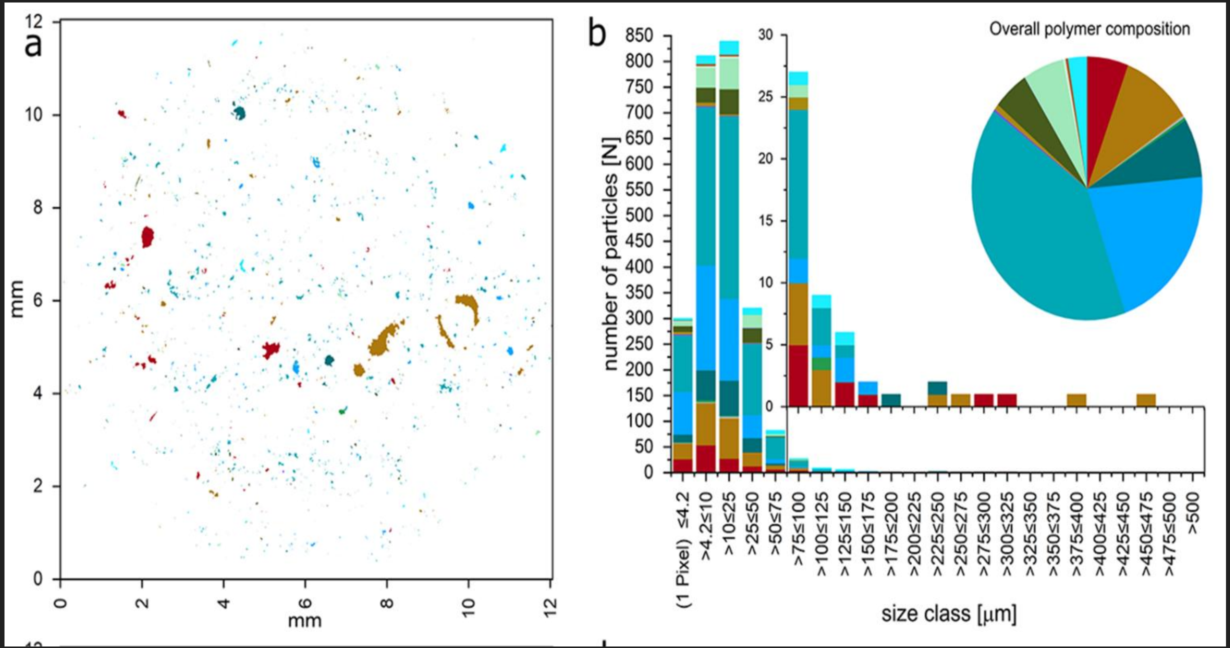
Classic spectral identification technique



Run a correlation between a known library spectra and unknown potential microplastic spectra

The Dream

We want automated spectroscopy to characterize microplastic shape, size, color, and polymer type.



Primpke et al. 2020

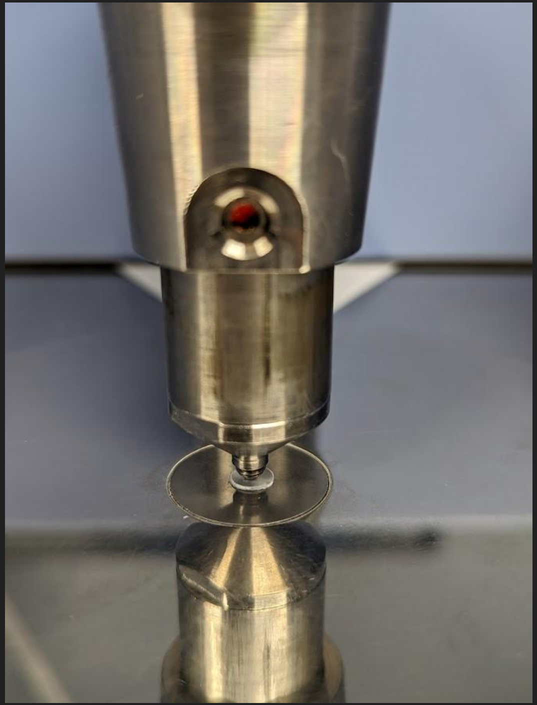
Before chemical analysis

How much should be characterized?

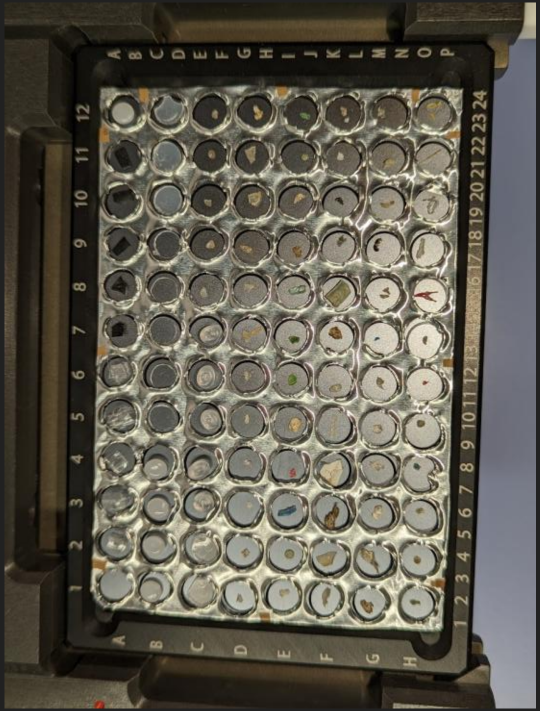
- It is recommended to analyze <u>AT LEAST</u> 100 randomized suspected microplastics, *Cowger et al. 2024*. Don't use percentage-based subsampling.

ATR is too slow! > 10 min per particle, IR Plate Readers may help

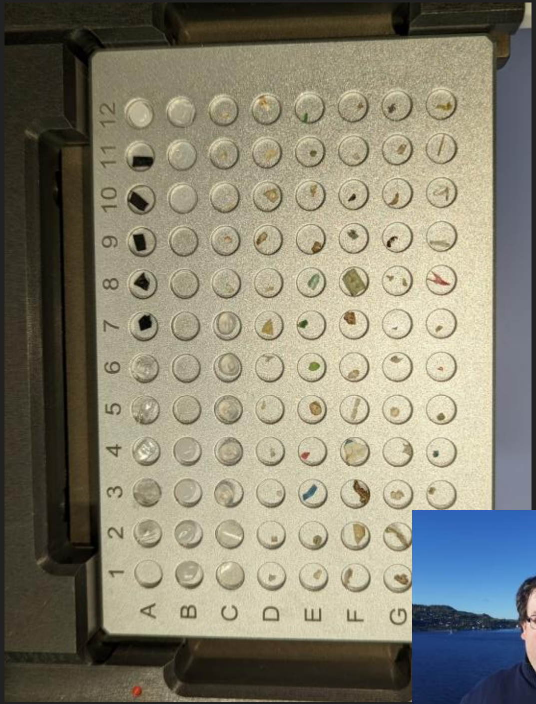
ATR



Transmission



Reflection

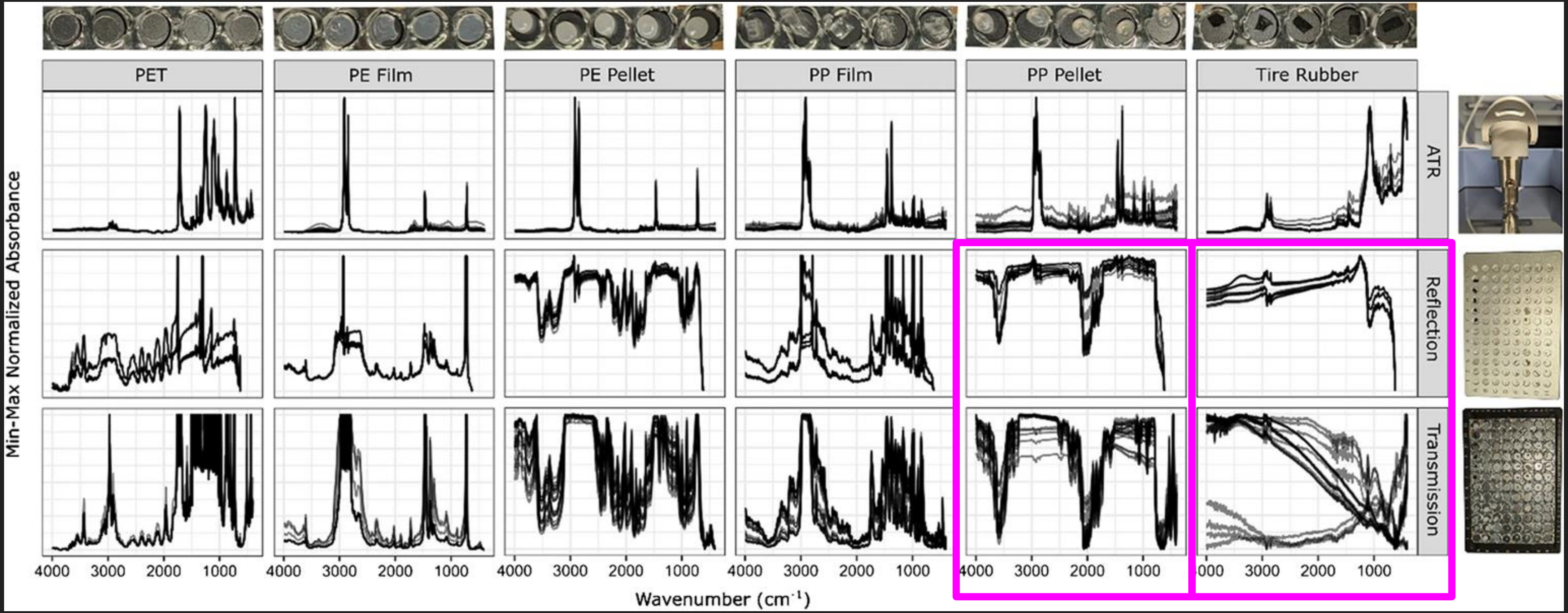


6k spectra collected of minerals, plastics, and organic materials

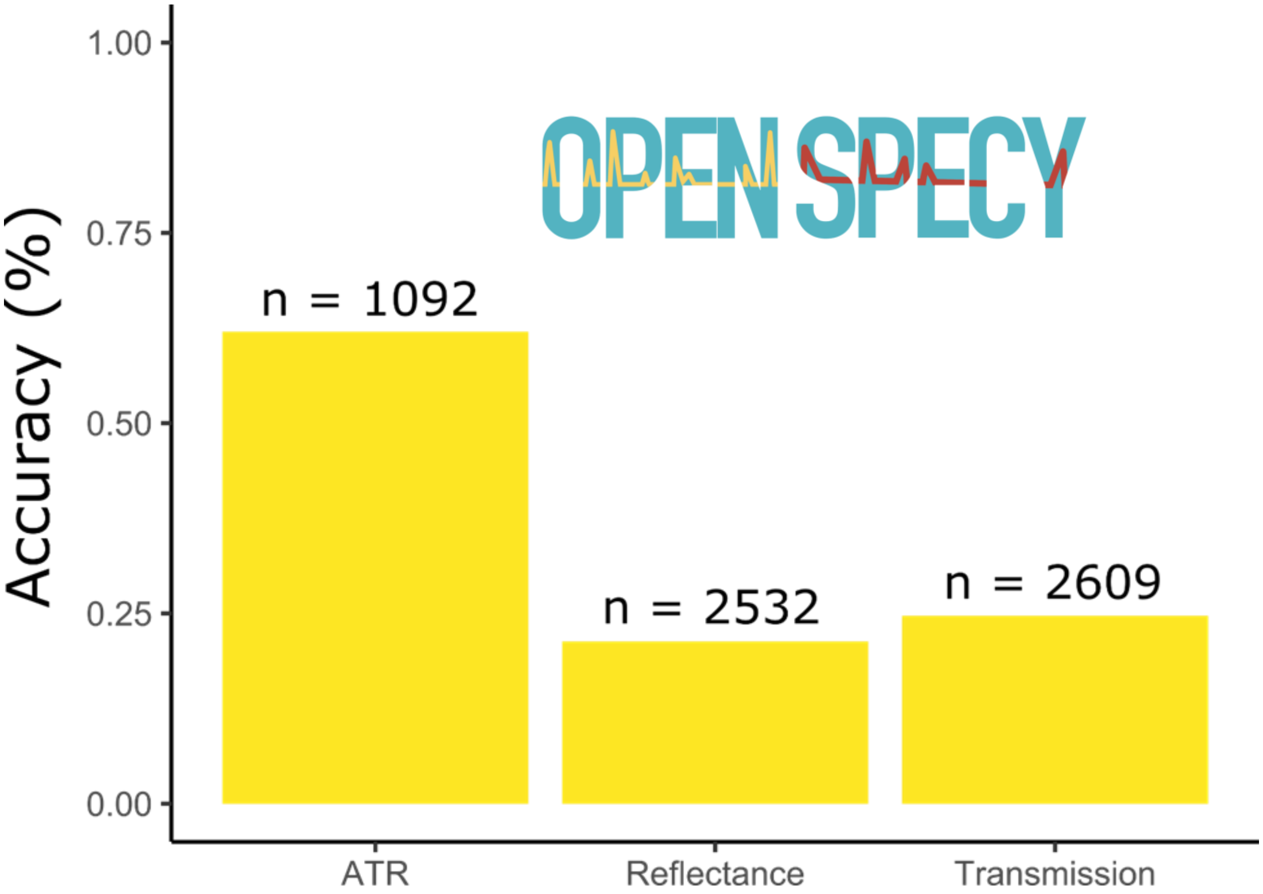
Sebastian Primpke

(FT)-IR plate reader challenges

Tire wear particles and thick particles have poor signal to noise



Known Issues



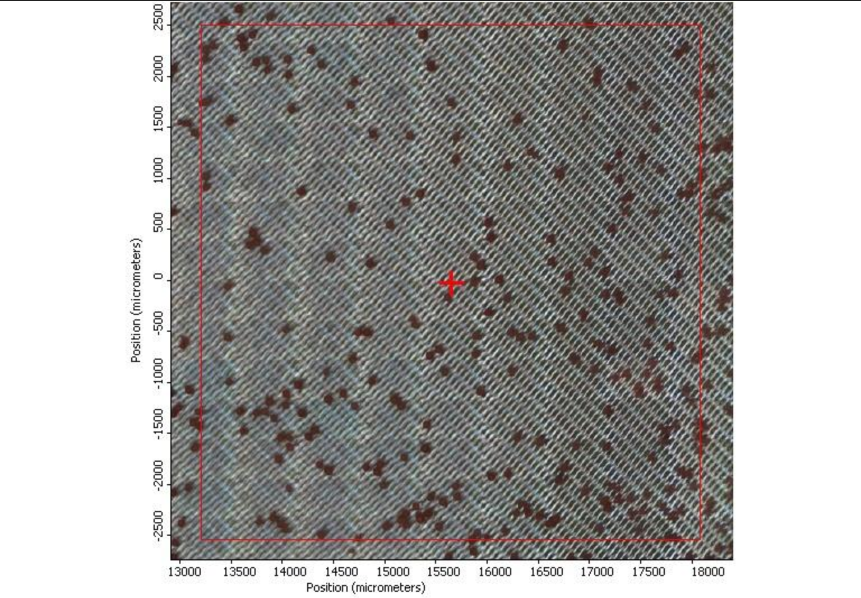
Databases can be inadequate if not built for purpose

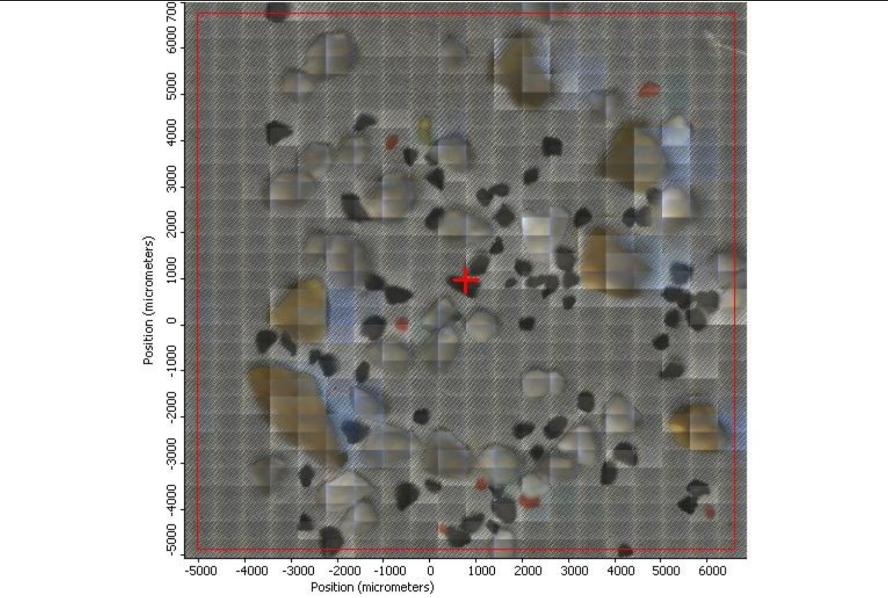
Out of the Box Accuracy was OK for ATR but lower for Reflectance and Transmission.

Cowger et al. 2024

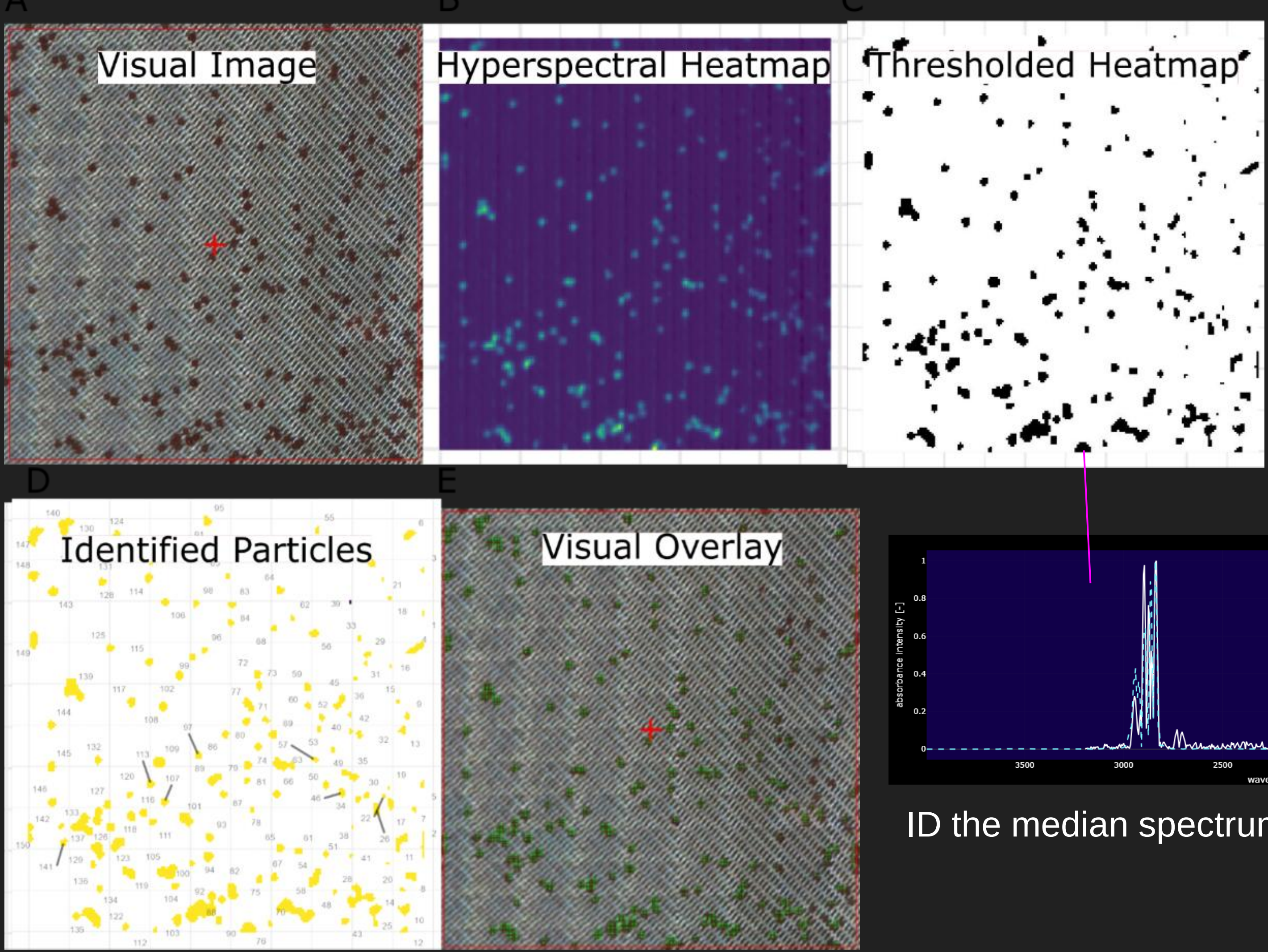
Testing Automated Hyperspectral Methods

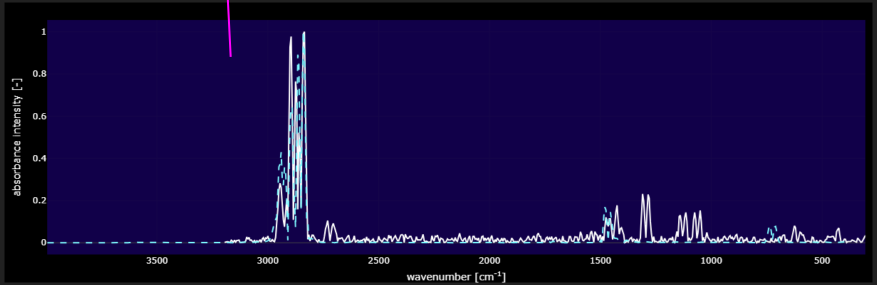
1. Homogeneous particles on a surface.
2. Did this for 20 different materials.





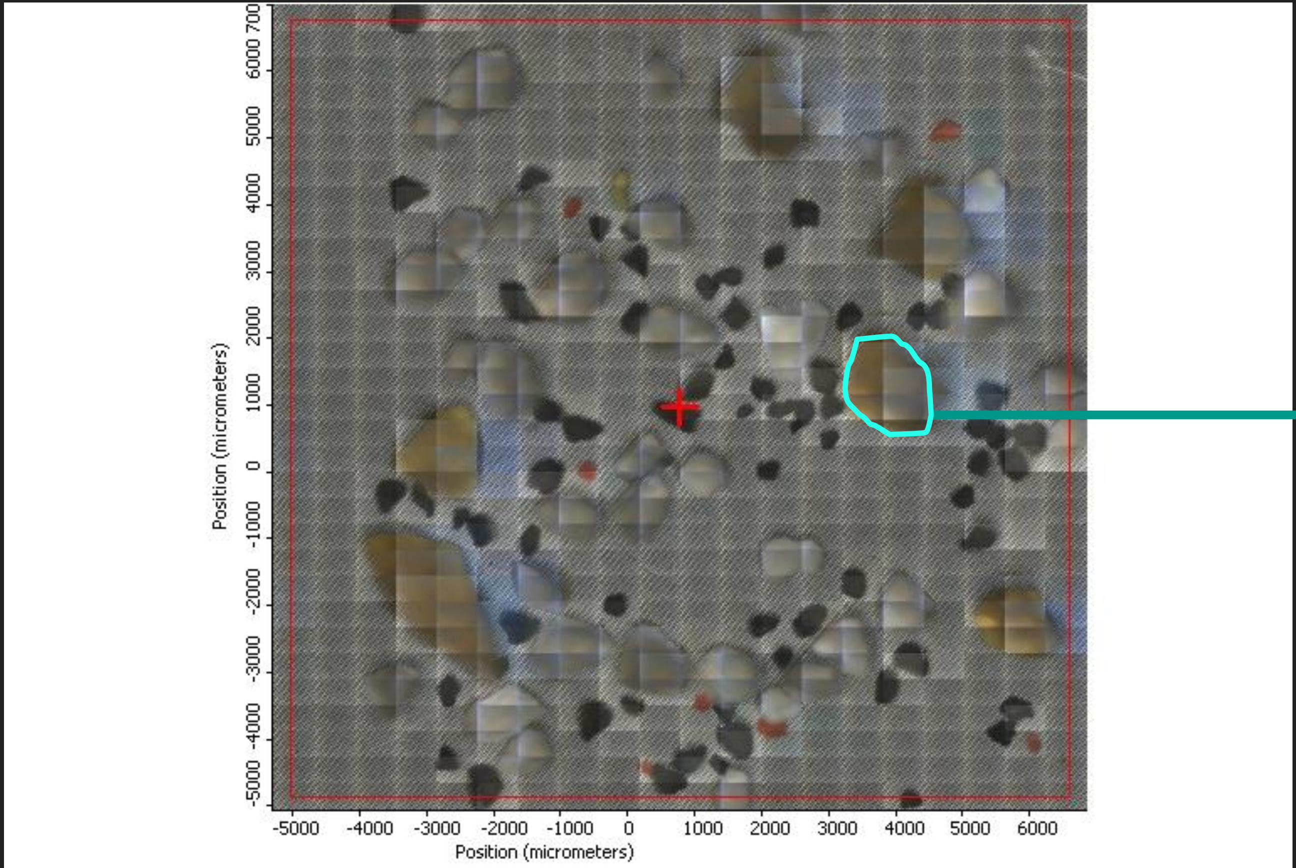
Testing Automated Methods





ID the median spectrum for each particle

Other Features

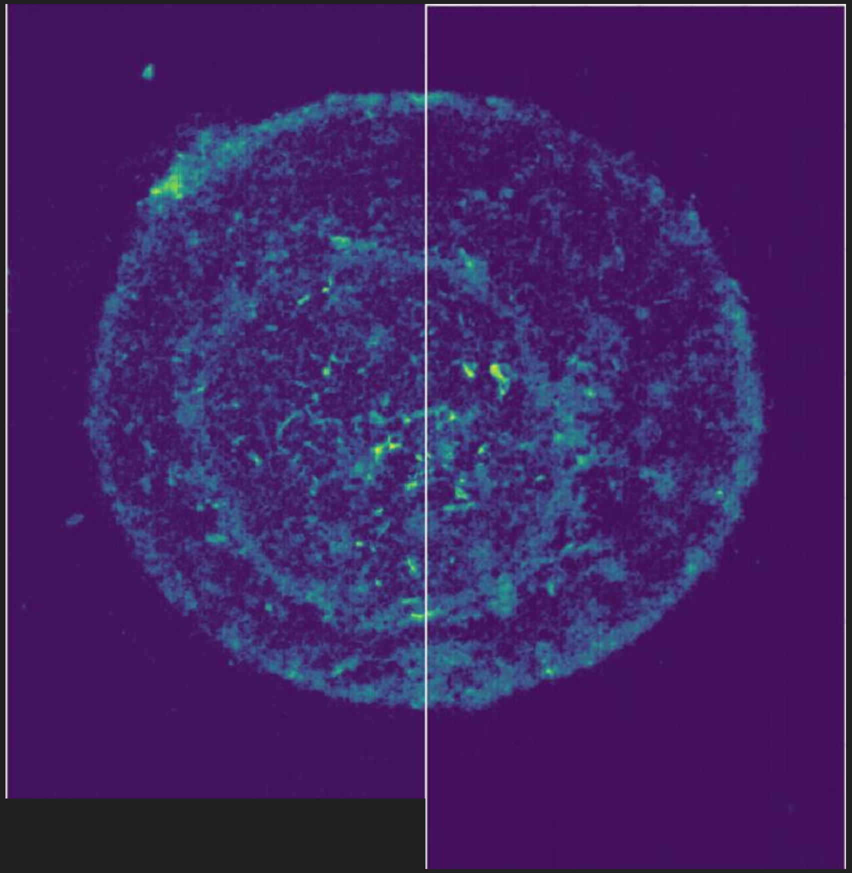


Overlay and extract average RGB colors

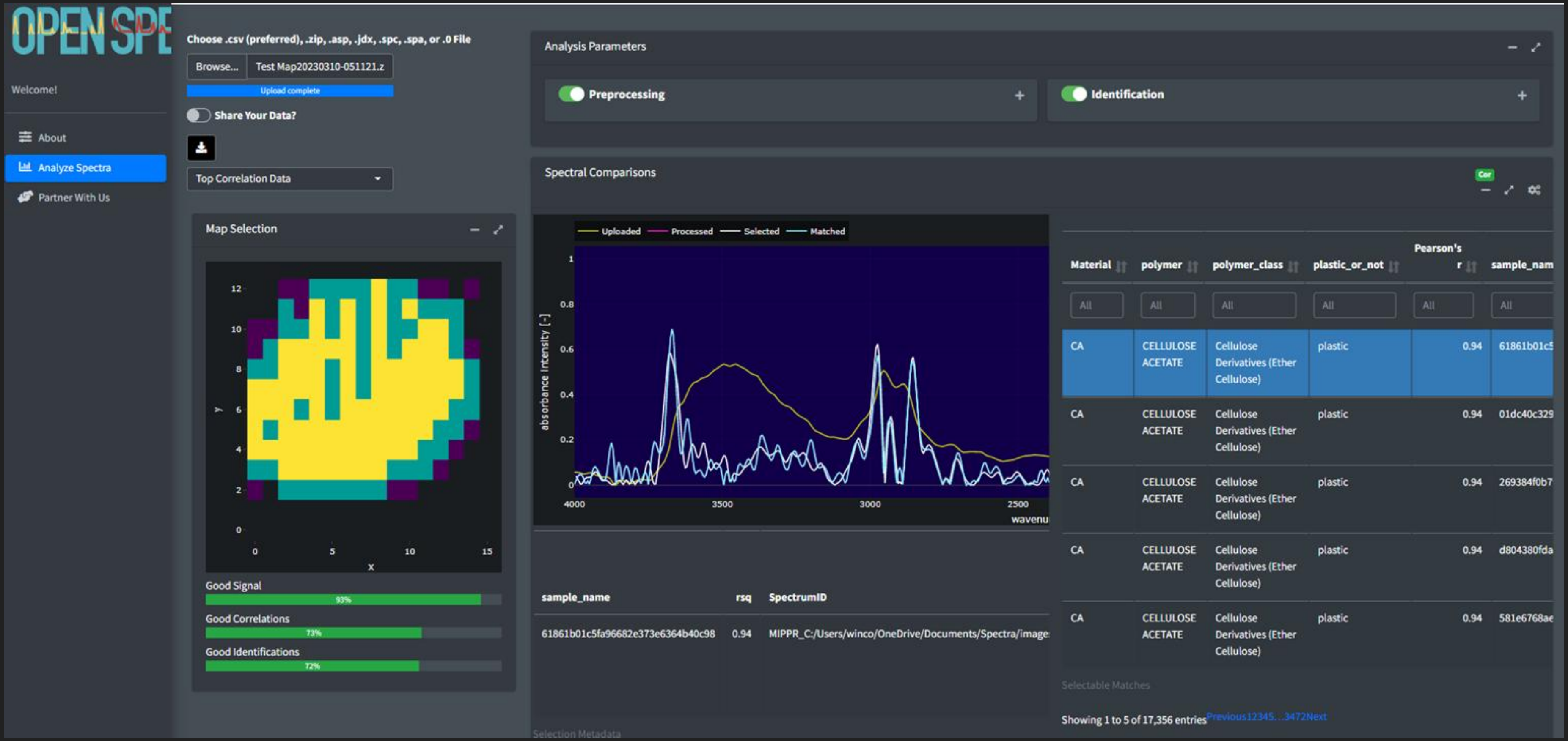
(255, 255, 0)

Other Features

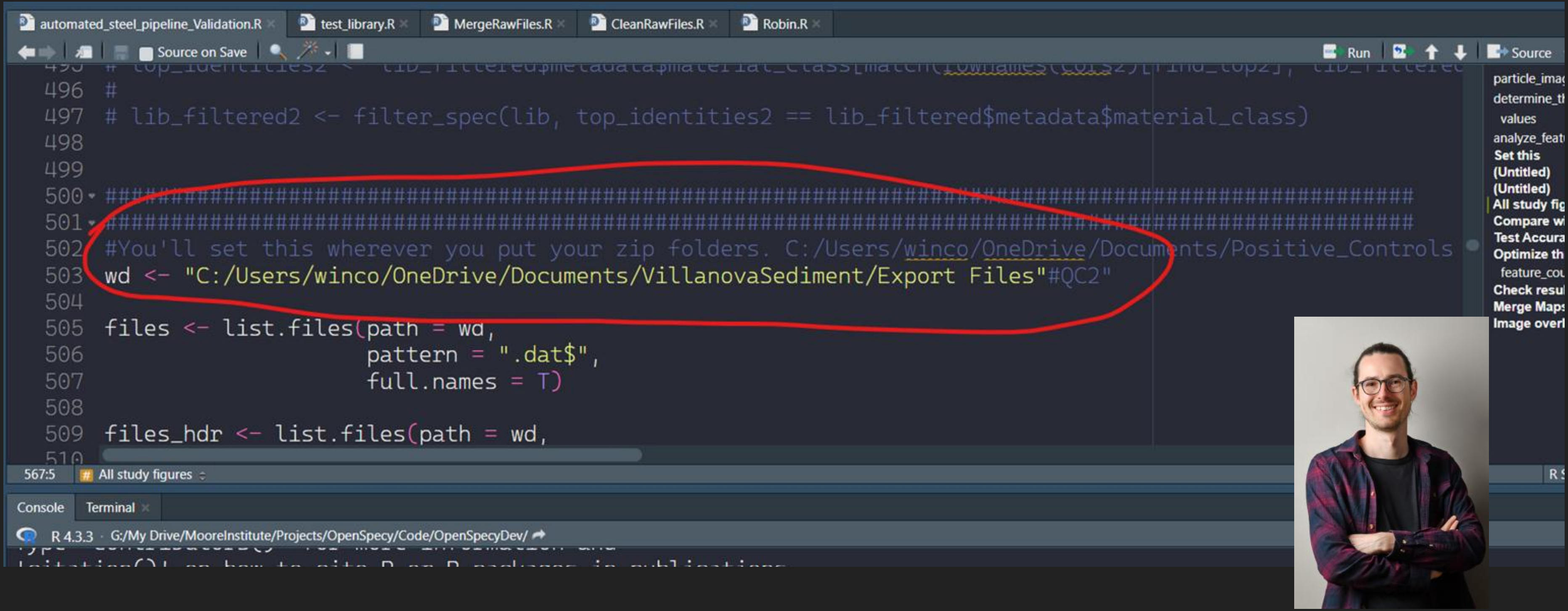
Stitching maps, you may not be able to map everything in one map



Open Specy online can do almost all of this but may be slow on large maps.



We can run everything in the Open Specy package by just changing a single line of code.



Zacharias Steinmetz

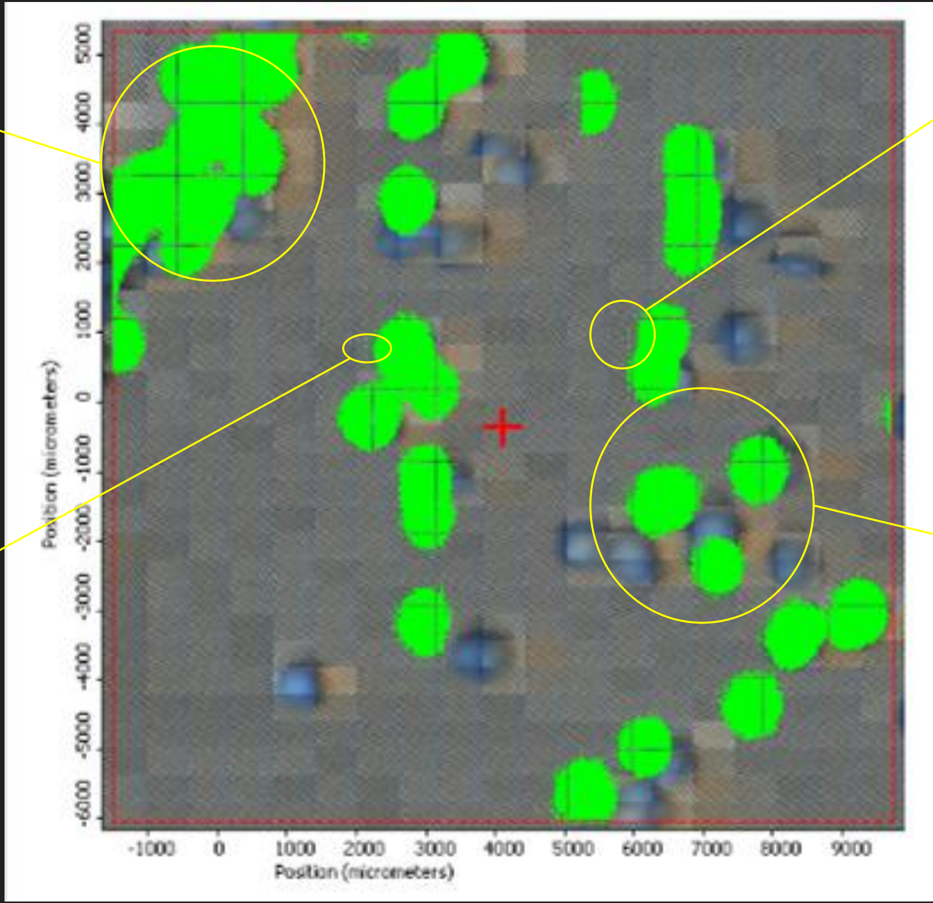
Current Metrics

1. Count Accuracy: 86%, RSD 34%
2. Identification Accuracy: 90%, RSD 24%
3. Size Accuracy: 94%, RSD 33%
4. Analysis Time: ~ 1 min for analyzing a 100k spectral map.
5. We are basically where we want to be but we must proceed cautiously.

Known Issues

Touching Particles Get Merged

Poor Signal Near Edges

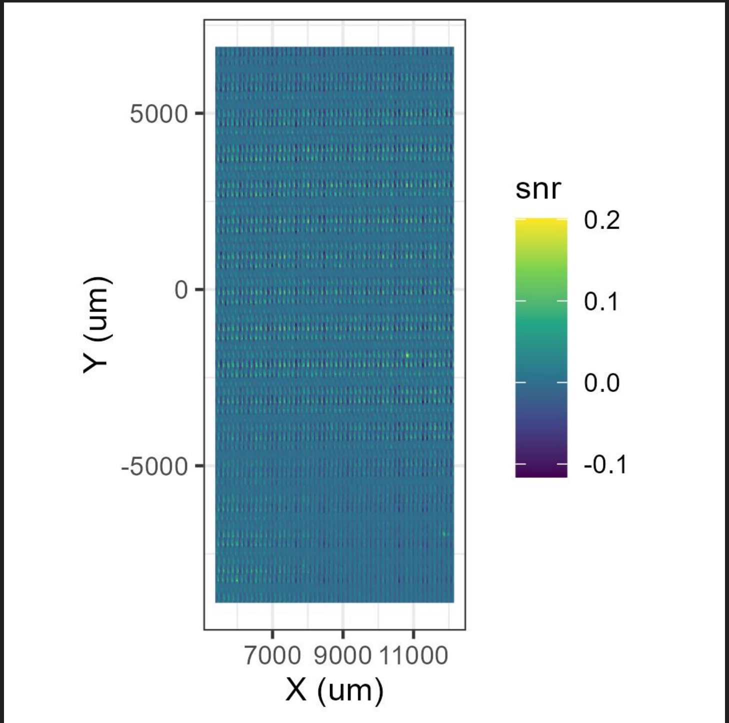


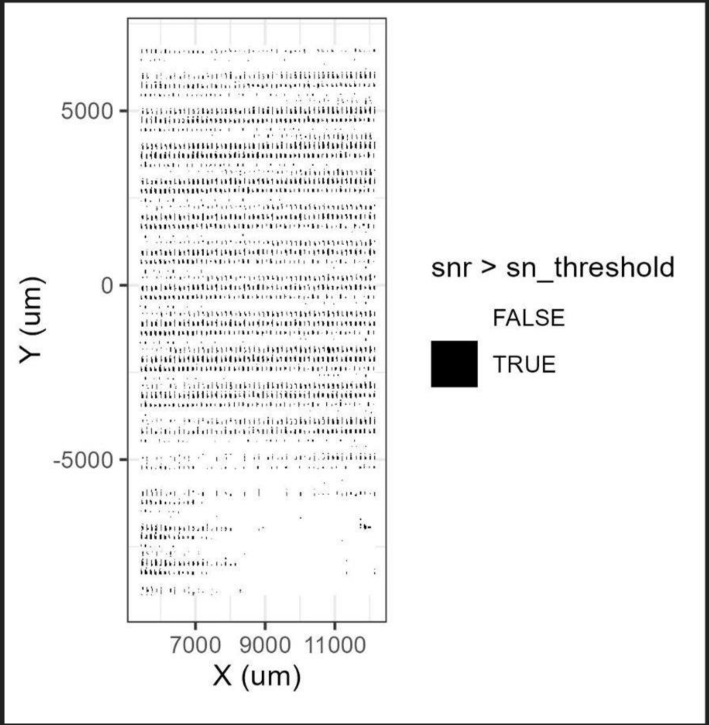
Ruptured particles at poor signal regions

Particles can move between visual and infrared imaging

Known Issues

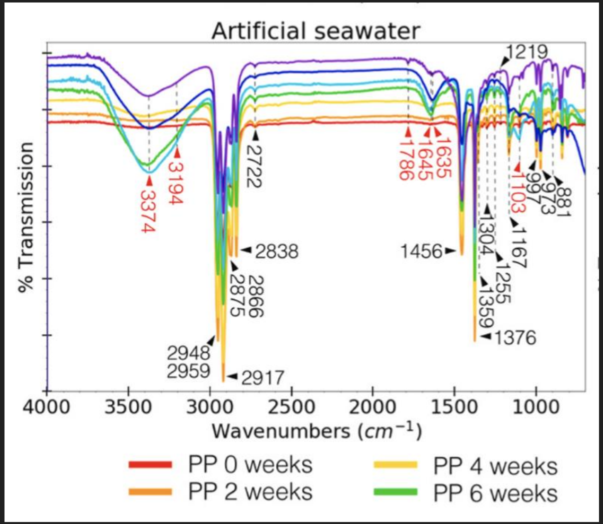
Inappropriate background, mesh size > step size, also the sample needs to be flat!





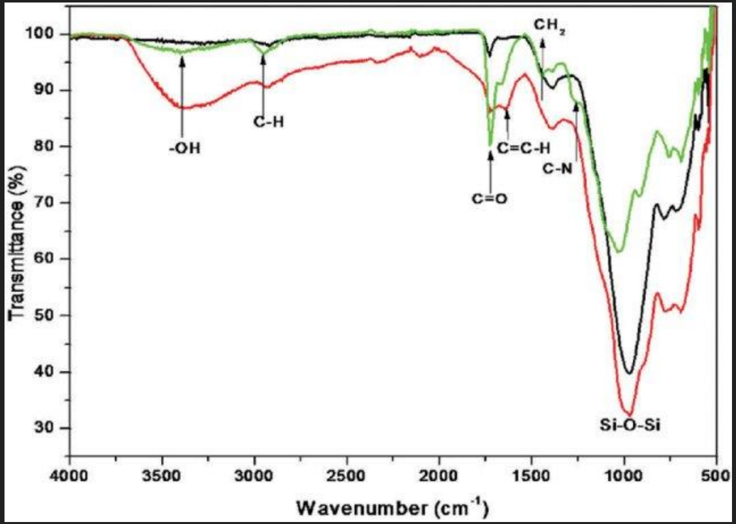
Challenges in identification

Weathering endows new spectral features



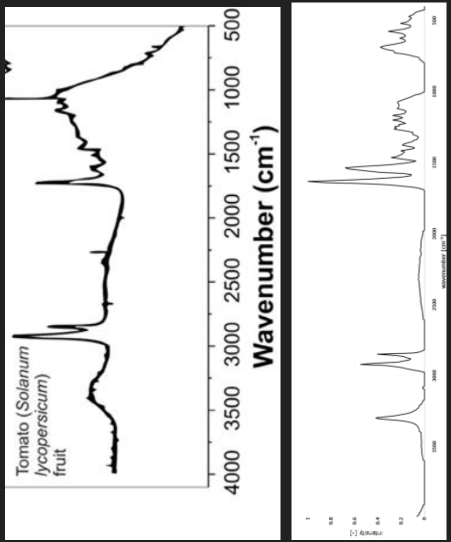
Phan et al. 2022

Mineral doped plastic has strong mineral signal



https://www.researchgate.net/publication/327803682_Functionalized_glass_fiber_membrane_for_extraction_of_iodine_species/figures

Natural and synthetic polyamides are very similar



Chamel and Maréchal (1992).

Next Steps

- New AI algorithm in collaboration with Monash University to use 500k reference library we developed.
- A new package for batch analyzing maps.
- New functionality for nanoplastic (< 1um) measurement with Raman imaging and leachate analysis with A-TEEM.

FTIR vs QCL-IR in Microplastics Characterization

Can We Achieve Consistent Results by Applying Similar Processing Steps?

Wesam Alwan, Ph.D.
Applications Scientist
Molecular Spectroscopy Division
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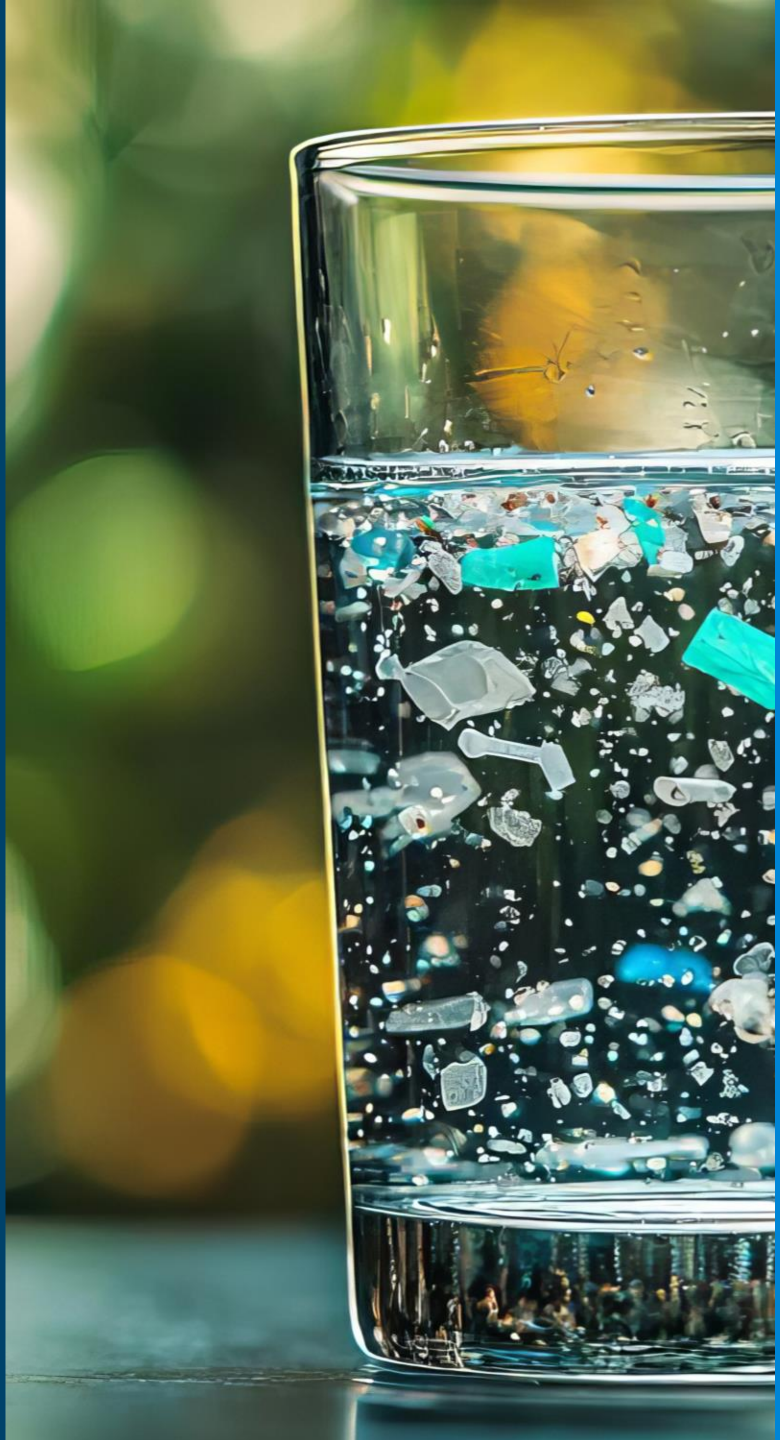

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The Question We Asked

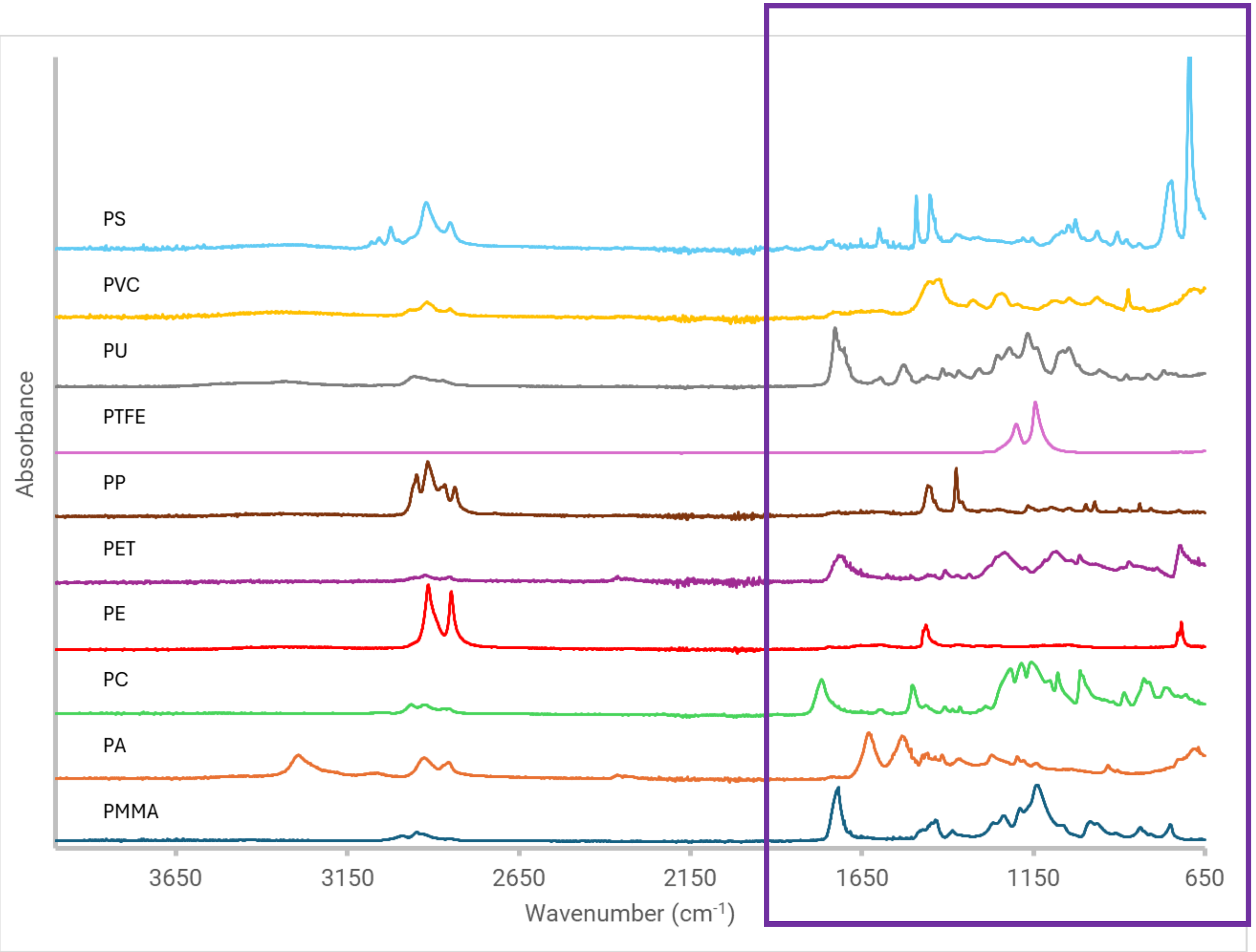
Wavenumber range | Optical design | Sample introduction substrates | Signal-to-noise ratio

Measurement mode | Library selection | Data processing methods

Since only a few aspects of testing variations can be controlled, such as sample introduction substrates, library selection, and data processing, an important question arises:

Can narrowing the **IR spectral range** impact the accuracy of microplastics identification?

Identifying Microplastics Using IR Spectroscopy



$1{,}260$ to $1{,}087$ cm−1 (CF_2 stretching vibrations)

$1{,}480$ to $1{,}400$ cm^{-1} (CH_2 bending vibrations)

$1{,}760$ to $1{,}670$ cm−1 (C=O stretching vibrations)

$1{,}800$ to $1{,}740$ cm−1 (C=O stretching vibrations)

$2{,}980$ to $2{,}780$ cm^{-1} (stretching vibrations of $CH/CH_2/CH_3$ groups)

Experimental Approach - Comparative Study of FTIR & LDIR Systems

Polymer samples

- PE
- PP
- PET
- PS
- PVC
- PA
-
-
-
-

Identification

- FTIR-ATR
- μFTIR imaging equipped with an FPA detector.
- QCL-IR

Data processing

- Exporting spectra
- Converting reflection data to

Reference Library

- siMPle library, containing 326 ATR spectra of commonly encountered

Matching algorithm

- Pearson's method (4 ranges)

Cary 630 FTIR-ATR

Cary 620 μFTIR imaging system

8700 LDIR Chemical Imaging System

Cary 630 FTIR-ATR

Polymer	650–3945 cm^{-1}	950–3590 cm^{-1}	1250–3590 cm^{-1}	975–1800 cm^{-1}
PS	**0.95** Polystyrene	**0.78** Polystyrene	**0.78** Polystyrene	**0.84** Polystyrene
PE	**0.81** Polyethylene_low_density	**0.81** Polyethylene_low_density	**0.81** Polyethylene_low_density	**0.82** Polyethylene_low_density
PET	**0.61** Poly(ethylene_terephthalate)	**0.54** Poly(ethylene_terephthalate)	**0.47** Fibre_polyester	**0.62** Poly(ethylene_terephthalate)
PC	**0.89** Polycarbonate	**0.90** Polycarbonate	**0.87** Polycarbonate	**0.91** Polycarbonate
PVC	**0.28** Poly(vinyl_chloride)_carboxylated	**0.30** Polyvinylchloride_with_plasticizer	**0.26** Polyvinylchloride_with_plasticizer	**0.60** Polyvinylchloride_with_plasticizer
PP	**0.79** Fibre_polypropylene_dyed	**0.80** Fibre_polypropylene_dyed	**0.80** Fibre_polypropylene_dyed	**0.94** Fibre_polypropylene_dyed
PTFE	**0.96** Poly(tetrafluoroethylene)	**0.97** Poly(tetrafluoroethylene)	**0.36** Poly(tetrafluoroethylene)	**0.98** Poly(tetrafluoroethylene)
PA	**0.51** Nylon_6_6	**0.51** Nylon_6_6	**0.50** Nylon_6_6	**0.72** Nylon_6_6
PU	**0.77** Polyurethane	**0.78** Polyurethane	**0.76** Polyurethane	**0.82** Polyurethane
PMMA	**0.85** Polymethyl methacrylate	**0.86** Polymethyl methacrylate	**0.83** Polymethyl methacrylate	**0.88** Polymethyl methacrylate

Correlation	<0.4	0.4 – 0.6	0.6 – 0.8	>0.8

All polymers were identified correctly

- **PTFE** performs best at 975–1,800 cm^{-1}.
- Fingerprint region improves correlation for **PA**, **PP**, and **PVC**.
- **PET** and **PS** show highest correlation in both full and narrow ranges.
- Minimal correlation variation for **PMMA**, **PC**, **PE**, and **PU** across all spectral ranges.

Cary 620 µFTIR imaging system

Polymer	650–3945 cm^{-1}	950–3590 cm^{-1}	1250–3590 cm^{-1}	975–1800 cm^{-1}
PS	**0.41** Polystyrene	**0.80** Polystyrene_expanded	**0.79** Polystyrene_expanded	**0.84** Styrene_acrylonitrile
PE	**0.41** Polyethylene_low_density	**0.61** Polyethylene_low_density	**0.63** Polyethylene_low_density	**0.69** Polyethylene_foamed
PET	**0.54** Polyethylene terephthalate	**0.63** Polyethylene terephthalate	**0.57** Polyethylene terephthalate	**0.63** Polyethylene terephthalate
PC	**0.37** Polycarbonate	**0.55** Polycarbonate	**0.60** Polycarbonate	**0.58** Polycarbonate
PVC	**0.17** Vinyl_chloride_vinyl_acetate_hydroxypropyl_acrylate	**0.38** Vinyl_chloride_vinyl_acetate_hydroxypropyl_acrylate	**0.38** Polyvinylchloride	**0.47** Vinyl_chloride_vinyl_acetate_hydroxypropyl_acrylate
PP	**0.62** Polypropylene	**0.71** Polypropylene	**0.70** Fibre_polypropylene	**0.88** Polypropylene
PTFE	**0.14** Polytetrafluoroethylene	**0.44** Polytetrafluoroethylene	**0.37** Poly(tetrafluoroethylene)	**0.67** Polytetrafluoroethylene
PA	**0.43** Nylon_6_6	**0.71** Nylon_6_6	**0.71** Nylon_6_6	**0.74** Nylon_6_6
PU	**0.46** Alkyd_varnish	**0.61** Alkyd_varnish	**0.70** Alkyd_varnish	**0.61** Alkyd_varnish
PMMA	**0.31** Polymethyl methacrylate	**0.38** Polymethyl methacrylate	**0.36** Polymethyl methacrylate	**0.39** Polymethyl methacrylate

Correlation	<0.4	0.4 – 0.6	0.6 – 0.8	>0.8

All polymers were identified correctly

- Full range shows lowest correlation due to low S/N at spectrum edges.
- 975–1,800 cm^{-1} improves correlation for **PP** and **PTFE**.
- **PA**, **PC**, **PE**, **PET**, **PMMA**, **PS**, **PU**, and **PVC** show minimal variation across ranges.

8700 LDIR Chemical Imaging System

Polymer	975–1800 cm^{-1}
PS	**0.94** Polystyrene
PE	**0.92** Polyethylene_low_density
PET	**0.82** Polyethylene_terephthalate
PC	**0.92** Polycarbonate
PVC	**0.74** Polyvinylchloride
PP	**0.96** Polypropylene
PTFE	**0.63** Polytetrafluoroethylene
PA	**0.90** Nylon_6_6
PU	**0.75** Polyurethane
PMMA	**0.73** Polymethyl methacrylate

Correlation	<0.4	0.4 – 0.6	0.6 – 0.8	>0.8

Using Pearson's correlation, LDIR data accurately identified all polymers.

Polymer	975–1800 cm^{-1}
PS	**0.978** Polystyrene
PE	**0.987** Polyethylene
PET	**0.954** Polyethylene terephthalate
PC	**0.953** Polycarbonate
PVC	**0.878** Polyvinylchloride
PP	**0.984** Polypropylene
PTFE	**0.976** Polytetrafluoroethylene
PA	**0.964** Polyamide
PU	**0.943** Polyurethane
PMMA	**0.952** Polymethyl methacrylate

Microplastics Starter 2.1 library and Clarity software accurately identified all polymers.

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Microplastics Analysis and the Infrared Spectrum: Is Spectral Range Selection Critical?

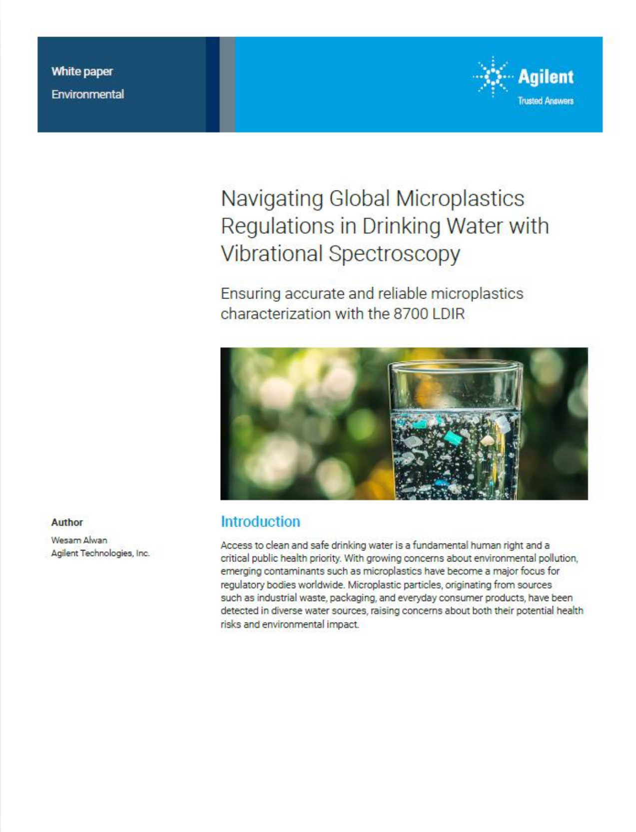
Authors
Wesam Alwan, Ciaran Worth, and Philip Wilson
Agilent Technologies, Inc.

Introduction

Microplastic contamination is an emerging threat to environmental and ecological systems across the globe. Microplastics are defined as small (less than 5 mm) solid fragments of synthetic or modified natural polymers that are insoluble in water.[1] Studies have shown that plastic particles cause harm to multiple types of organisms through exposure to toxic substances.[2,3] Despite these known toxic effects, the full extent of the impact of microplastics remains unclear due to challenges in developing reliable methods for characterizing this broad class of micro-sized polymers.

Infrared (IR) spectroscopy is an established technique for characterizing microplastics. It identifies the molecular composition and structure of materials by measuring the absorption of IR radiation. The resulting absorption bands, which are due to intramolecular vibrational modes, help identify organic or mineral materials through comparison of spectra with a library of spectra from known polymers.[1] Current directives and standard methodologies require that major types of polymers are identified correctly and can be distinguished from other natural materials.[1,4]

Microplastics Analysis and the Infrared Spectrum: Is Spectral Range Selection Critical?
5994-8037EN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Navigating Global Microplastics Regulations in Drinking Water with Vibrational Spectroscopy

Ensuring accurate and reliable microplastics characterization with the 8700 LDIR

Author
Wesam Alwan
Agilent Technologies, Inc.

Introduction

Access to clean and safe drinking water is a fundamental human right and a critical public health priority. With growing concerns about environmental pollution, emerging contaminants such as microplastics have become a major focus for regulatory bodies worldwide. Microplastic particles, originating from sources such as industrial waste, packaging, and everyday consumer products, have been detected in diverse water sources, raising concerns about both their potential health risks and environmental impact.

Navigating Global Microplastics Regulations in Drinking Water with Vibrational Spectroscopy
5994-8166EN