

CHEMINFORMATICS AND HYPERSPECTRAL IMAGING FOR ILLICIT DRUG INTELLIGENCE: TOWARD A STANDARDIZED FRAMEWORK FOR NPS AND COMPLEX MIXTURE ANALYSIS

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*8th International Conference on Frontier in Diagnostic Technologies
Frascati, October 19th 2026*



This project has received funding from the European Union's HORIZON EUROPE innovation programme under grant agreement No. 101168195

An Illicit drug Crime Scene can be anywhere

Clan-LAB



<https://www.hampshirealert.co.uk/Alerts/A/365272/Investigation-launched-following-discovery-of-large-cannabis-factory-in-Farnborough>

Small Pills



<https://antidroga.interno.gov.it/schede/mdma/>



Cultivation Facility

How to handle?

<https://www.europol.europa.eu/media-press/newsroom/news/24-industrial-scale-labs-dismantled-in-largest-ever-operation-against-synthetic-drugs>



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even smaller than you can imagine... e or so small...



[Credits Elijah Pilchard](#) on [Unsplash](#)



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Nitazenes and fentanyl derivatives can be part of that fine particle



Active principle	Dose/effect [to morphine]
Heroin	2–4×
Fentanyl	50–100×
Nitazenes (general)	500–1,000×
Isotonitazene (ISO)	500×
Etonitazene	1,000×
Protonitazene	~500×
Metonitazene	~200–300×
Carfentanil	10,000×
Acrylfentanyl	~400×
3-Methylfentanyl	~1,500×
Acetylfentanyl	~50–100×



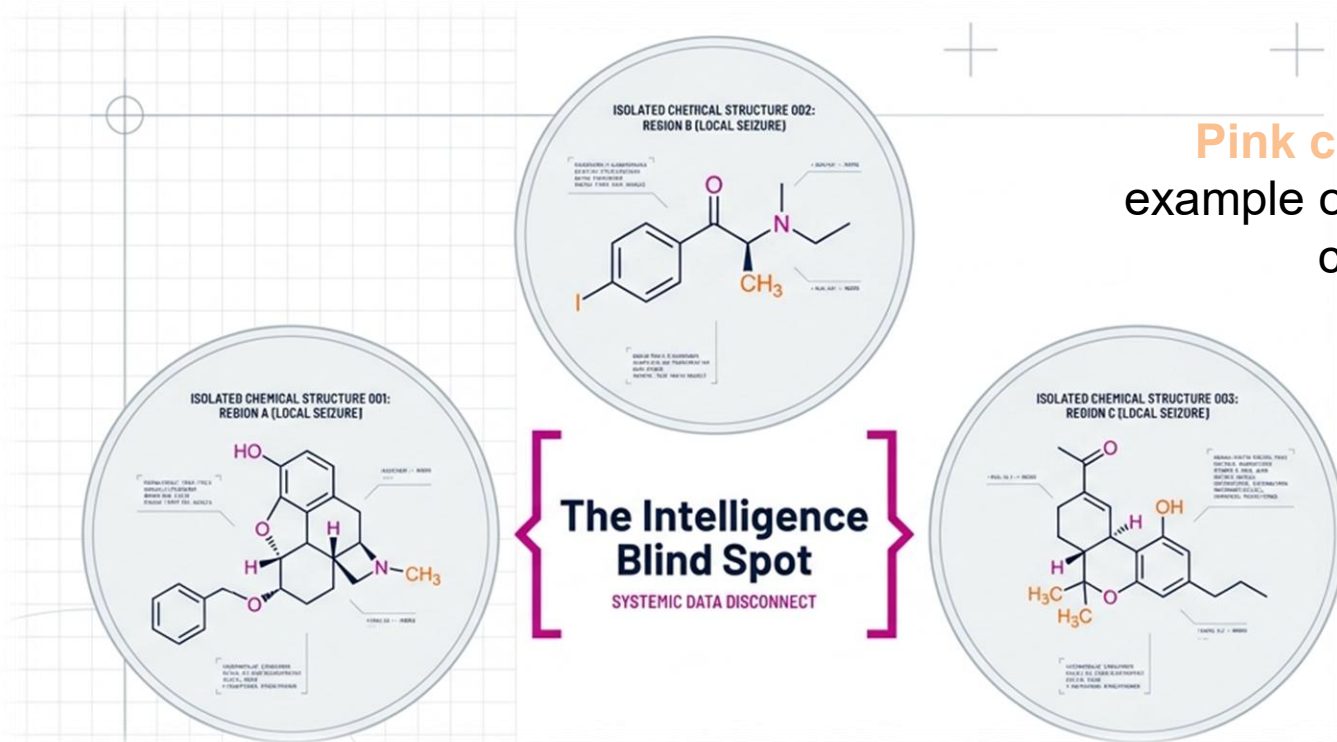
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From Seizure Data to Strategic Intelligence:

break the professional silos that prevent LEAs from seeing the 'big picture' of illicit drug trafficking



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Pink cocaine is a good
example of how a street name
can mislead



ketamine and MDMA
rather than cocaine



Break the Chemistry professional silos



Eliminating Naming Confusion: Why We Need a Unified Naming Tool



docker

Fuzzy logic
RESTful
microservice



Incorrect Name
to
Correct Name

Naming & Structure Linkage Service

Swagger UI for the Naming & Structure Linkage Service.

default

- GET /v1/resolve_ikey Resolve ikey
- GET /v1/check_ikey_exists Check ikey Exists
- POST /v1/reload Reload References
- GET /health Health
- POST /v1/search_by_formula Search By Formula
- POST /v1/normalize Normalize json

Parameters: No parameters

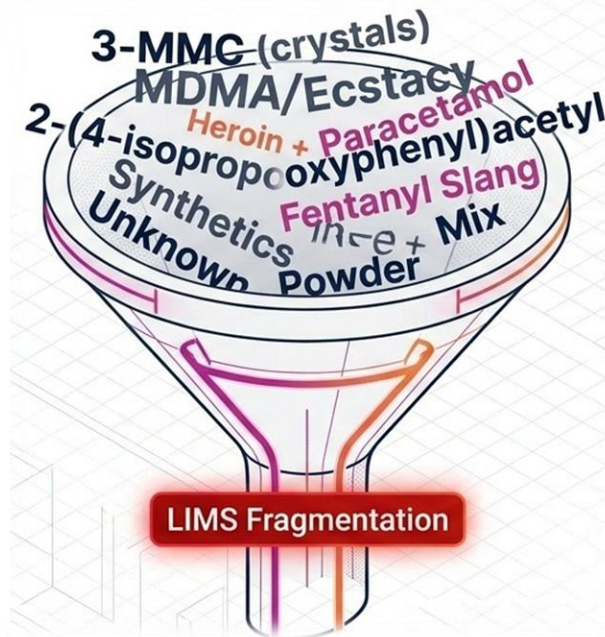
Request body **required**: application/json

Example Value | Schema

```
{  "name": "string",  "ikey_score": 0,  "unique_only": true,  "top_n": 1}
```

Responses

Code	Description	Links
200	Successful Response	No links



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Naming & Structure Linkage Service



NARCOSIS Spectroscopy NARCOSIS Workbench Interactive

Peak selection is slider-based for stability: choose a point with the slider, then add the optional label and store the peak.

[Compound Archive](#) FT-IR / RAMAN GC-MS NMR MS Library Search FT-IR Library Search

Chemical Identification & Formulation Intelligence

Case Record Selection

Search records

Search by record ID, report number, molecule, etc.

Search **New record** **Read selected record**

Selected record_id: 5

Export to PDF **Upload Word Template** **Record loaded: 5**

Exported PDF

Drop File Here
or
Click to Upload

Save Template

Word Template Path:

Records

record_id	numero_scheda	molecola	classe	formula	localita
1	N.1001	2-HMC	catinoni sintetici	C10H15NO	Roma
2	N.1002	3-HMC	catinoni sintetici	C10H15PMO	Parigi
3	N.1003	3-MEC	catinoni sintetici	C12H17NO	Lisbona
4	N.1004	3-HMC	catinoni sintetici	C10H15NO	Madrid
5	N.1005	4F-NPH	stimolanti sintetici	C14H18PMO2	Berlino
6	N.1006	Benzazepam	benzodiazepine	C14H10O5N3O	Vienna
7	N.1007	Clonazepam	benzodiazepine	C15H10ClN3O3	Praga
8	N.1008	Cocaine	cocainici	C17H21NO4	Milano
9	N.1009	MDA	fenetilamine	C10H13NO2	Amsterdam
10	N.1010	MDMB-4en-PINACA	cannabinoidi sintetici	C20H28N4O3	Bruxelles
11	N.1011	MDMB-PINACA	cannabinoidi sintetici	C19H28N4O3	Aterre
12	N.1012	MDA	fenetilamine	C10H13NO2	Amsterdam

Case Details & Evidence

General Case Information

Record Images

Upload/Modify Images

Standardizing Forensic Expert reporting to NFP

A new pipeline to feed NPS names into a simple, exchangeable CSV list

canonical_iupac_name	smiles	localized	compound_class	synonyms	street_names	formula	inchikey	inchi	pubchem
2-AI		2-AI	Aminoindanes	2-aminoindane		C9H11N	LMHHFZA	InChI=1S/	76310
MDAI		MDAI	Aminoindanes	5-methylenedioxy-2-aminoindane		C10H11NC	FQDRMH	InChI=1S/	125558
5-IAI		5-IAI	Aminoindanes	5-iodo-2-aminoindane		C9H10IN	BIHPYCDD	InChI=1S/	131506
MDMAI		MDMAI	Aminoindanes	N-methyl-2-aminoindane		C11H13NC	KNZKMF	InChI=1S/	125559
LA-111		LA-111	Aminoindanes			C16H13Cl	AAOVKJB	InChI=1S/	3016



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Naming & Structure Linkage Service

The «formulation» concept



Reference Library Management

Save Target
Compound 1
Save Current Compound to Master Reference Library

Intelligence Workspace

Search Criteria

Molecule Name
3-mec

Molecular Formula
e.g. C17H21NO4

Match Threshold Score
Lower = more candidates, Higher = stricter matches
80

Search Local Library Search by Formula External Search

Identification Candidates

canonical_name	iupac_name	formula	compound_class	pubchem_cid	inchikey	inchi
3-mec	2-(ethylamino)-1-(3-methylphenyl)propan-1-ol	C12H17NO		9169619	GEKLDQKEZAPF-UHFFFAOYSA-	InChI=1S/C12H17NO/c1-4-13-10(3)12(14)11-7-8-5-6

Verification & Enrichment

Target Slot
Main Compound

Class Override
Aminoidanes

Enrich Selected Candidate

Pink cocaine ≠ cocaine: the street name reflects color/branding, not composition; most samples contain little or no cocaine. It is instead related to the formulation

The tool allows a search:

- Online on PubChem
- Locally by name or Brute Formula

Can search the so called formulation: A street name is associated to active principle+ cutting agent+physical aspect

Intelligence Workspace

Template Intelligence

Save as Formulation Template

Search Street Name
e.g. The Boost

Search Formulations

Enrich Formulation

Formulations Library

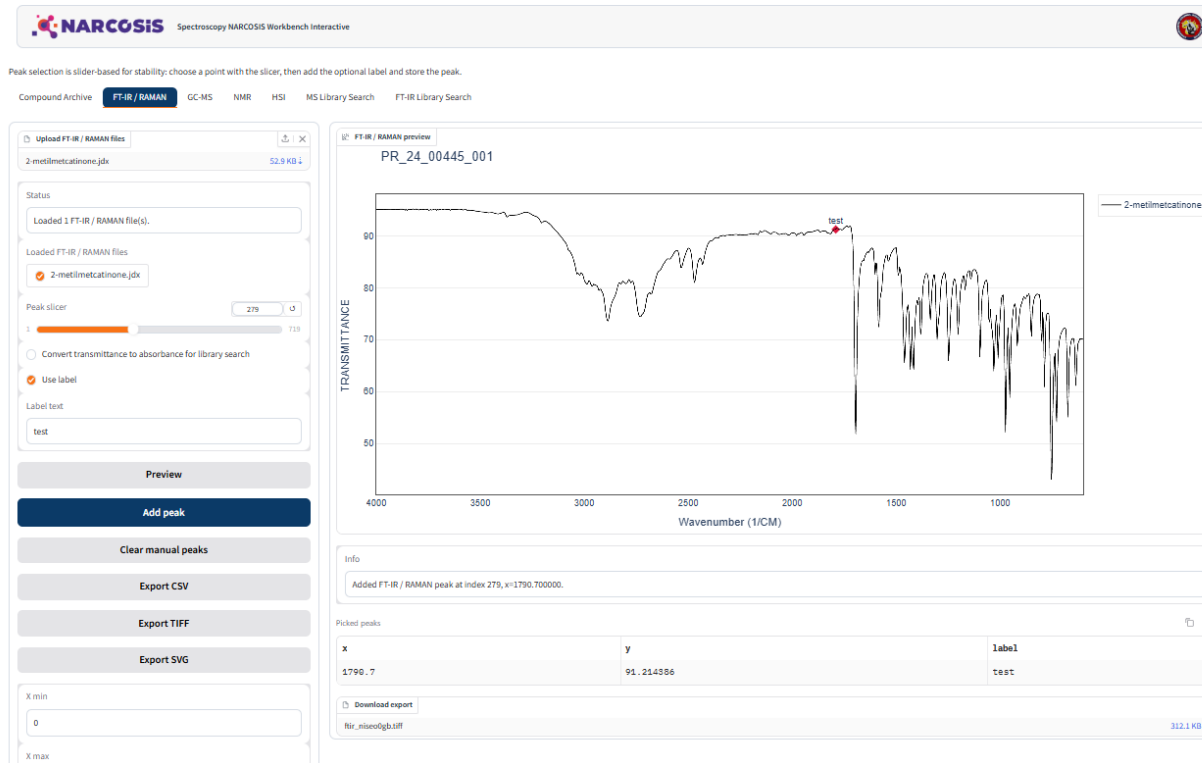
formulation_id	street_name	appearance
Selected ID		



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Naming & Structure Linkage Service

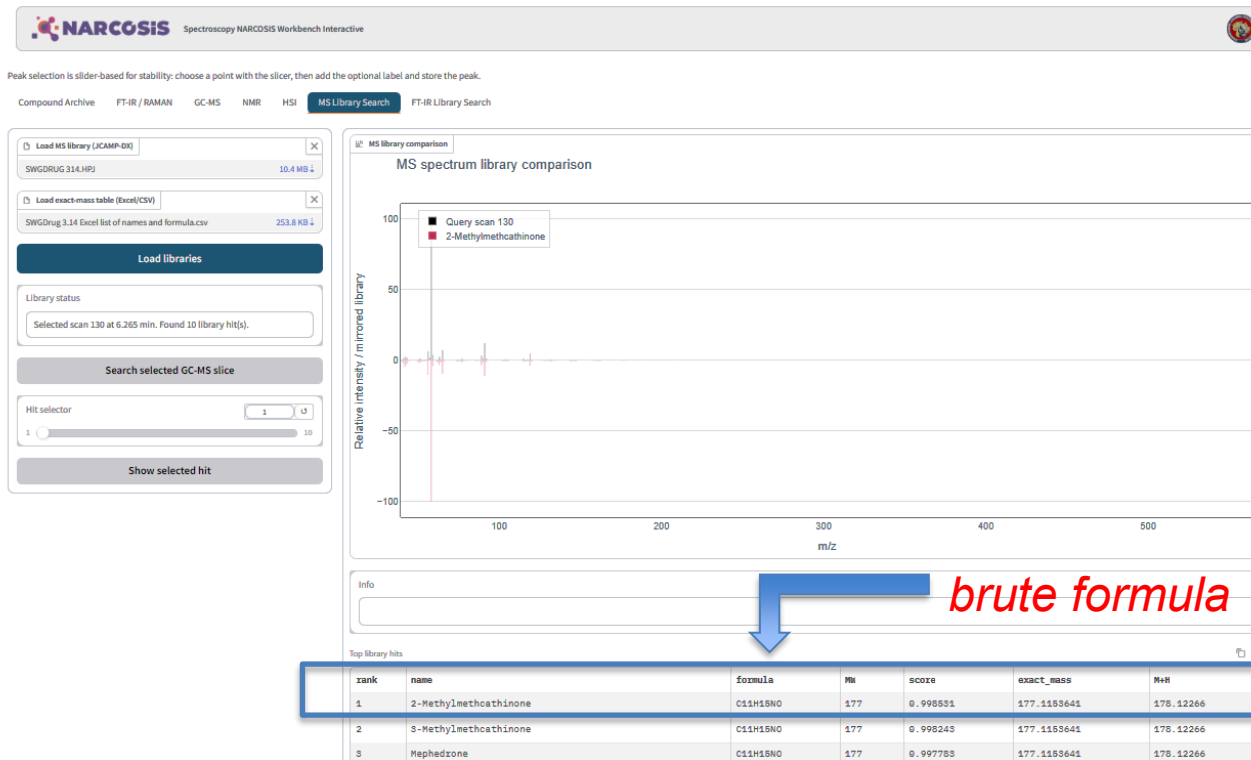
«Import» brute formula (FT-IR)



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Naming & Structure Linkage Service

«Import» brute formula – library search



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Naming & Structure Linkage Service

Investigate structural related compound



Spectroscopy NARCOSIS Workbench Interactive



Peak selection is slider-based for stability: choose a point with the slider, then add the optional label and store the peak.

Compound Archive **Compound Discovery** FT-IR / RAMAN GC-MS NMR HSI MS Library Search FT-IR Library Search

Explore

Select or Search Compound

2-MMC

Filter by Class

All Classes

☐ Auto-calculate pathway (predict metabolites/precursors)

Explore Lineage

Status

Success

Manage Relationships

Parent Compound

Child Compound

Molecular Lineage View

Precursors (select to add)

Predicted Precursors

Add Selected Precursors

Name	Type	Confidence
------	------	------------

Target Compound

Compound Details

Compound: 2MMC
Class: Other substances
Formula: C11H15NO
InChiKey: PRGXFAWAMOFULD-UHFFFAOYSA-N

Chemical Structure

Metabolites (select to add)

Predicted Metabolites

Add Selected Metabolites

Name	Type	Confidence
------	------	------------

Structural Relatives

Structurally Similar Compounds

Name	Similarity
2-Ethylethcathinone	86.9
4-MMC	66.6
Mephedrone-d3	66.6
N,N-Dimethylcathinone	66.2
N-ethylcathinone	65.8

Chemical Analysis

Triplet Plot / Structural Comparison



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REPORT to EUDA

ST14

 EUDA EUROPEAN UNION DRUGS AGENCY	
Report ID: ST14_2024_IT_02	
STANDARD TABLE 14: POTENCY/PURITY OF ILLICIT SUBSTANCES	
1. NOTES POTENCY/PURITY OF ILLICIT SUBSTANCES	
1.1. Notes on how to fill in Standard Tables	
Please note: Rules that have to be followed if the copy and paste from spreadsheet is to work.	
2. IDENTIFICATION INFORMATION	
2.1. Year, source and coverage	
Fill in one report for each routine statistic or ad-hoc study providing data on purity/potency of illicit d	
2.1.1 Data year	
2010	
2011	
2012	
2013	

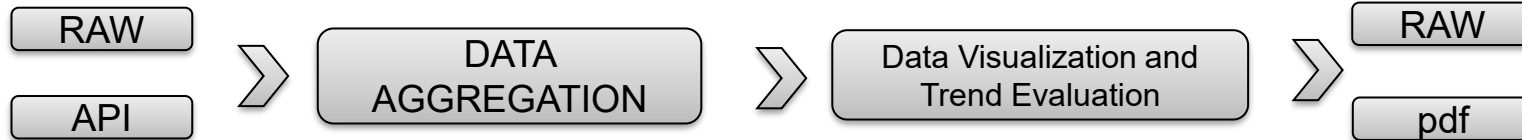
ST15

 EUDA EUROPEAN UNION DRUGS AGENCY	
Report ID: ST15_2024_IT_01	
STANDARD TABLE 15: COMPOSITION OF ILLICIT DRUG TABLETS	
1. NOTES COMPOSITION OF ILLICIT DRUG TABLETS	
1.1. Notes on how to fill Standard Table	
Notes on how to complete Standard Table 15: General notes 1Provide data on the contents of illicit drug tablets from as many sources as possible. Notes related to the Sample: - The number of records refers to the number of different tablet types analysed. - The number of table Substances: Scheduled drugs refer to substances controlled under the 1971 UN Convention on Psychotropic Substances Schedules I and II and unde	
2. IDENTIFICATION INFORMATION	
2.1. Year, source and coverage	
Fill in one report for each routine statistic or ad-hoc study providing data on composition of illicit drug tablets (do not include data from different sources)	
2.1.1 Data year	
	2010
	2011
	2012
	2013
	2014
	2015
	2016
	2017



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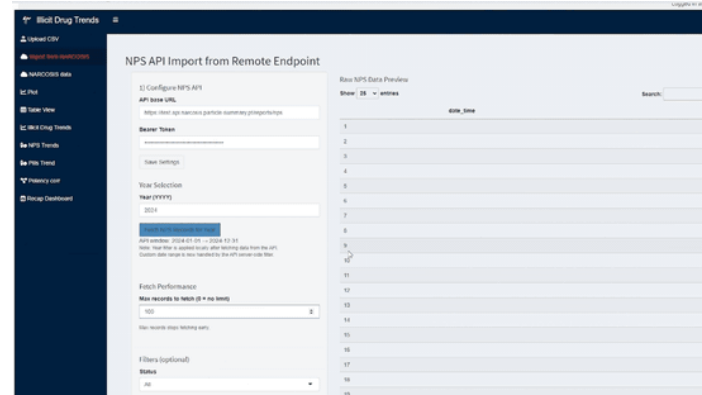
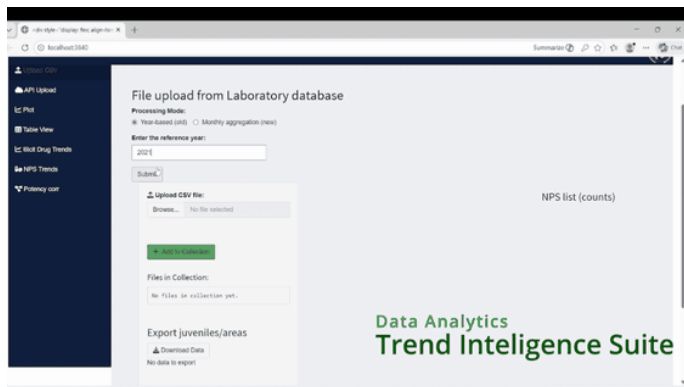
Trend Analysis Suite



Enable rapid, standardized monitoring of illicit drugs and emerging NPS across provinces and time, turning heterogeneous lab/seizure inputs into actionable trends.

Raw CSV

Raw API



Streamline early-warning reporting by automating data harmonization and producing consistent, export-ready outputs aligned with NEWS/EWS workflows



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Trend Analysis Suite: NPS Name Normalization

A screenshot of a web browser displaying the "NPS Naming Tool" interface. The browser's address bar shows "localhost:3840". The interface has a light blue background. On the left, there is a sidebar with several sections: "Regions" with buttons for "Alessandria", "Ancona", "Brescia", "Chieti", and "Foggia"; "Time aggregation" with radio buttons for "Yearly" (selected) and "Monthly (if available)"; "Select year(s)" with a text input containing "2024"; a checked checkbox for "Facet by Region" and a "Refresh" button; "Name normalization" with an orange "Normalize names" button and a checked checkbox for "Use canonical names in filters/plots"; and a "Map" section with a "Map period (year)" dropdown set to "2024" and a "Show labels" checkbox. The main content area has a title "Raw NPS results (rank 1 only, debug)" and a "Show 25 entries" dropdown. Below this is a table with columns: "input", "canonical_final", "compound_class", "match_method", "match_score", "pubchem_cid", and "formula". A search bar is located at the top right of the main area. At the bottom center of the interface, the text "NPS Naming Tool" is displayed in a large, bold, red font.

**Geospatial Analysis
Driven by Standardized
Compound
Classifications**



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Bridging the gap:

From Spectra of Chemicals to Chemical Spectral Images



- Tiny amount of illicit drug
- Molecular structure quite spread across several classes
- Psychoactive substances may be hidden into fabric or textiles

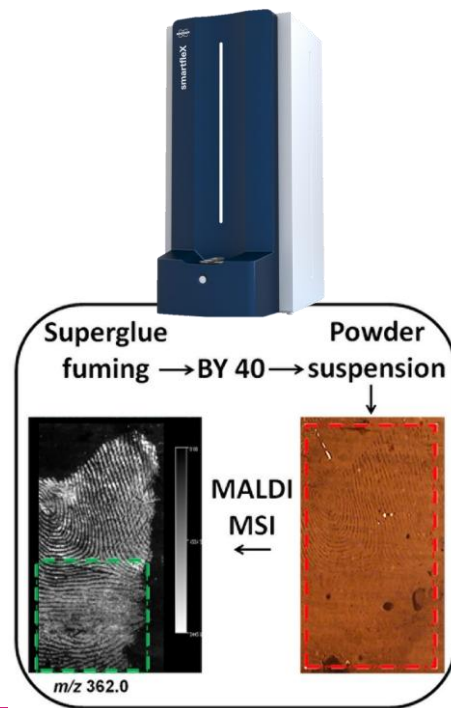
We started the software validation with blood then we will move to Illicit drugs



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Back to the crime scene

Chemical methods for latent trace visualization



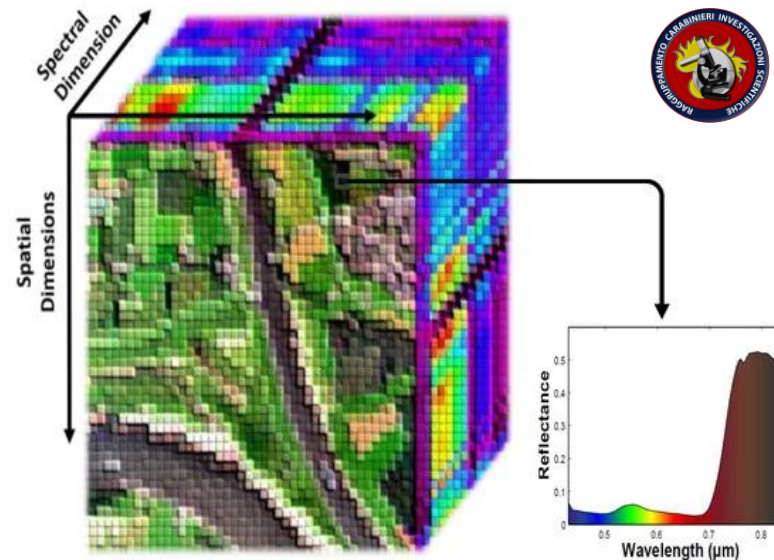
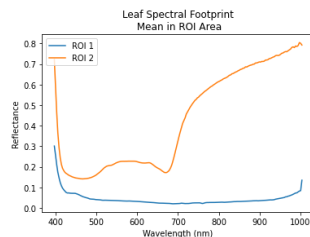
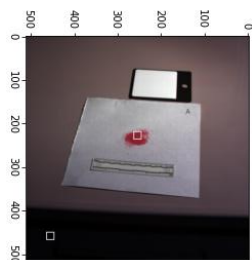
Physical methods for latent trace visualization



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Hyperspectral Imaging:

Specim IQ Hyperspectral Camera

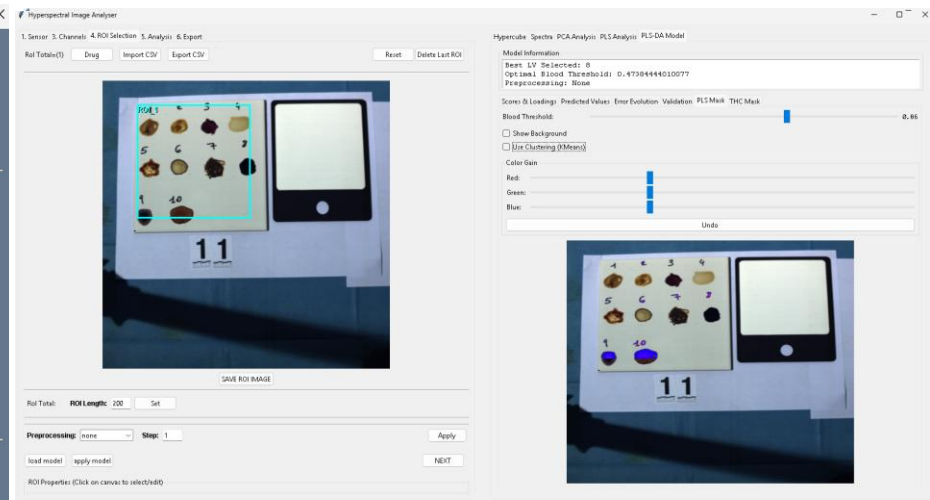


Spectral region of interest extraction (ROI)



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CSIAalyzer software



Previous version (left) vs New Version (right)



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Our experience:

Blood is hardest to see on dark or patterned substrates “stealth traces”

Dark

Black textiles and plastics absorb light, so the stain and the background look alike

Patterned

Coloured or textured surfaces hide traces and confuse colour-based cues

Reflective

Glass and metals add glare and specular artefacts that mask the stain

Practical

Practitioners need a non-contact, non-destructive way to decide where to sample



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CSIAalyzer: two complementary views

PCA — explore

- Unsupervised, first three PCs mapped to RGB
- Highlights spatial anomalies and suppresses the background
- Colours reflect spectral variance, not identity of the trace

PLS-DA — target

- Supervised model of the blood signature (Q-bands near 540 and 576 nm)
- Continuous score map; operator adjusts the display threshold
- Locates candidate traces for immunochromatographic tests

The aim is visualization and triage, not identification of blood.



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Experimental design

13

substrates: textiles, plastics,
metals, glass, mineral and
cellulosic

10

traces: equine blood (undiluted,
1:1 diluted) and 8 look-alikes

204

Max VNIR channels, portable
sensor, halogen illumination

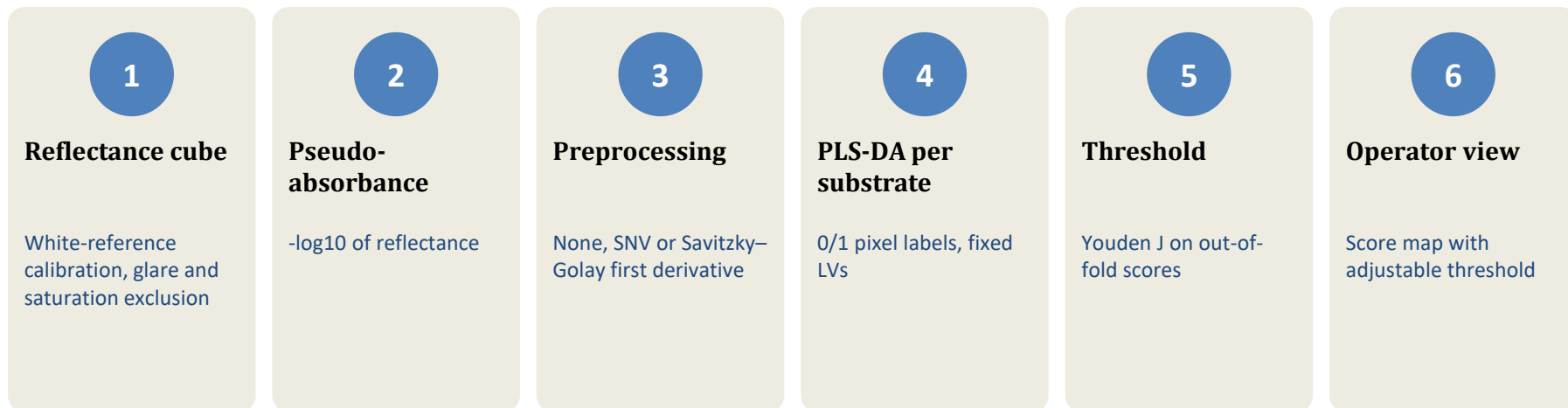
Two independent sessions

- TRACCE: training session, labelled ROIs of blood, look-alikes and background
- TRACCE_BIS: external session, different illumination and stain geometry, one image per substrate
- Look-alikes: ketchup, BBQ sauce, lipstick, red wine, tomato sauce, coffee, chocolate, synthetic blood
- Pixel counts reflect spatial sampling, not independent replicates



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Analysis pipeline



The same score map feeds the display threshold slider and an optional K-Means refinement.



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Three layers of validation

1

ROI-grouped 5-fold CV

Each ROI predicted by a model that has not seen it. Descriptive: ROIs of one stain are adjacent, so it reflects within-image separability.

2

Leave-one-substrate-out

12 substrates train, the 13th tests. Used to fix the number of latent variables per preprocessing, and as a cross-substrate score check.

3

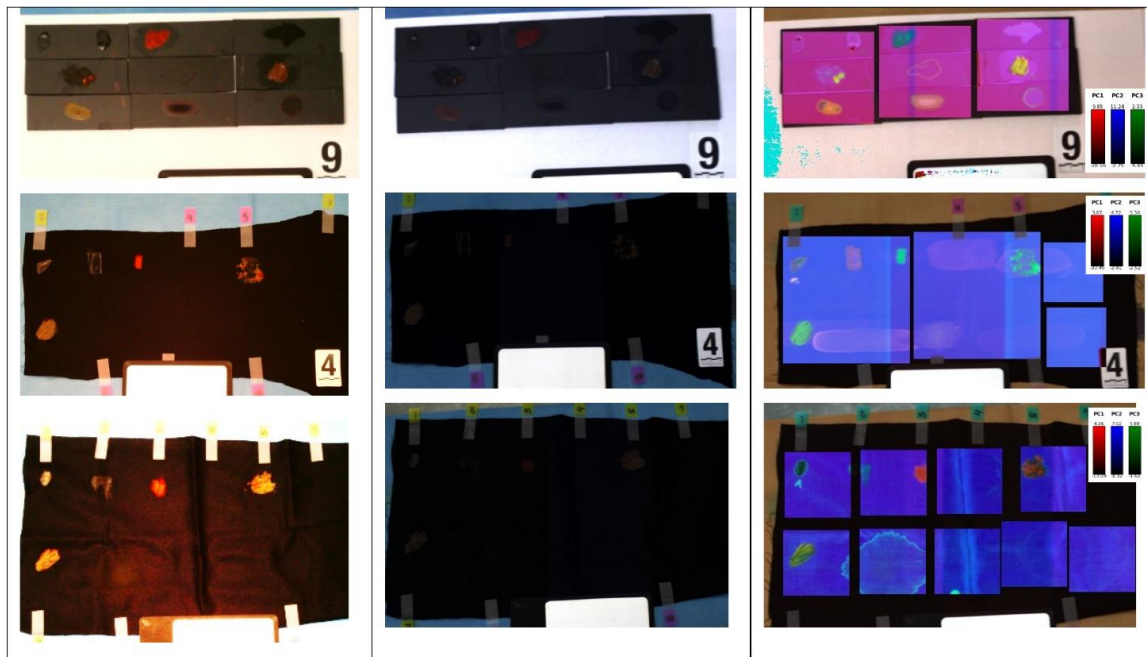
External session

Frozen models with frozen thresholds on TRACCE_BIS: new session, new illumination, new stain geometry.



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PCA reveals traces on dark substrates

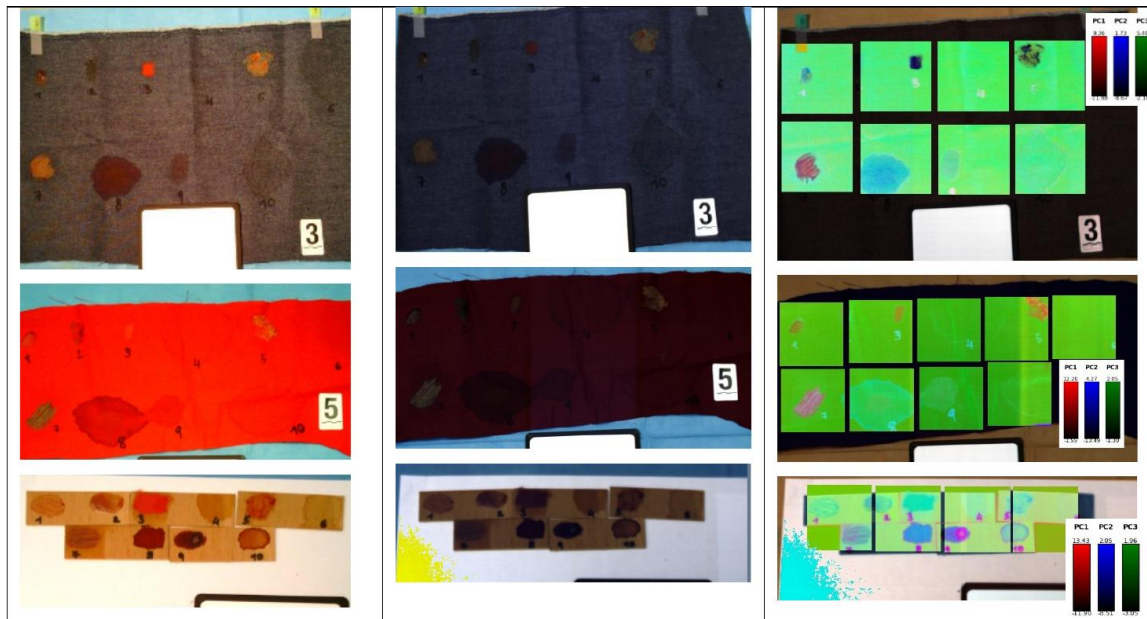


- RGB photographs show little or nothing on black cotton, polyester and PVC
- PCs 1–3 mapped to RGB expose the stains
- Undiluted and moderately diluted blood is clearest
- On black polyester, diluted samples diffuse into the fabric: the practical detection limit



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Coloured and textured substrates



- Red dye (S5) absorbs 500–550 nm, overlapping the oxyhaemoglobin Q band
- Indigo (S3) adds a broad slope at 600–650 nm
- Lignin (S13) gives a rising absorbance toward the blue
- Background optical properties interfere with the blood signature



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Reflective surfaces and glare

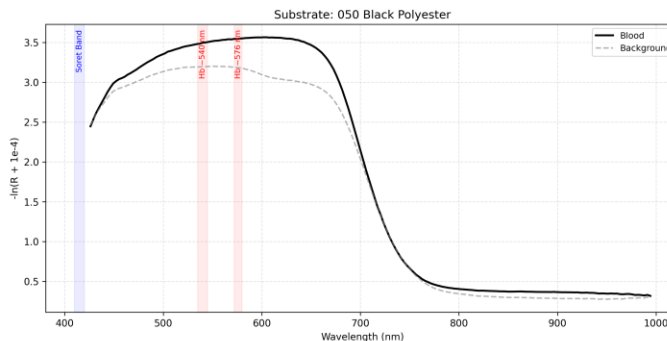
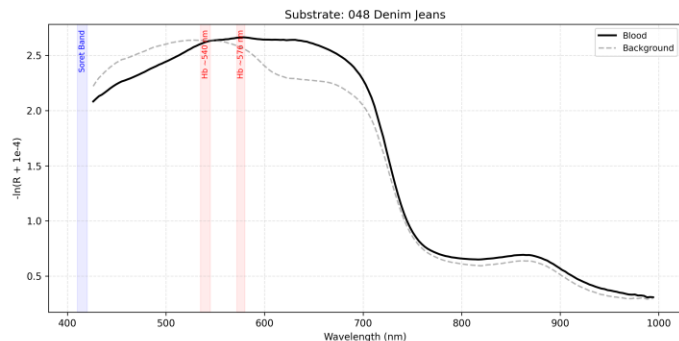
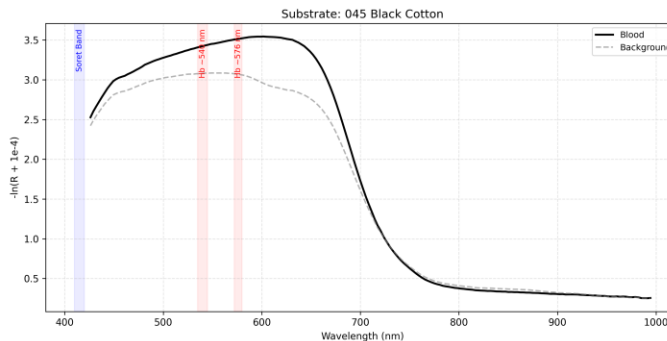
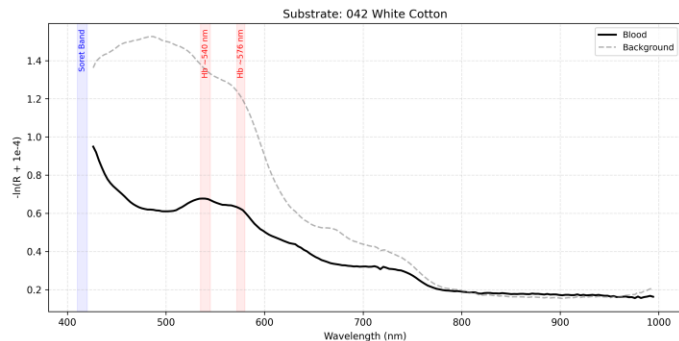


- Specular reflections and glare dominate the RGB images and can saturate the detector
- In the cube, geometric artefacts are separated from the chemistry
- Traces are mapped on aluminium, steel and glass



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Spectra: the blood signature and its distortion

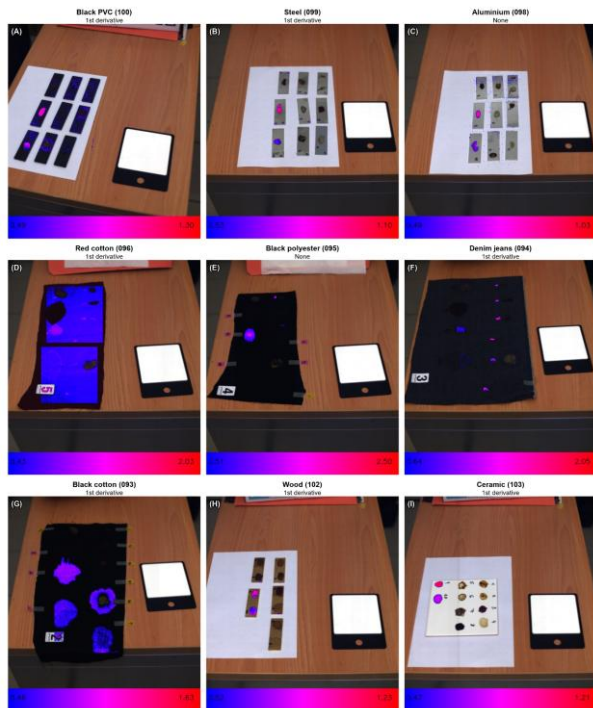


- Blood carries the Q-band doublet at 540 and 576 nm
- Background co-absorption and substrate properties distort the raw spectra
- Simple thresholding or manual wavelength selection cannot classify blood across dark or chromatic surfaces
- This motivates supervised PLS-DA modelling



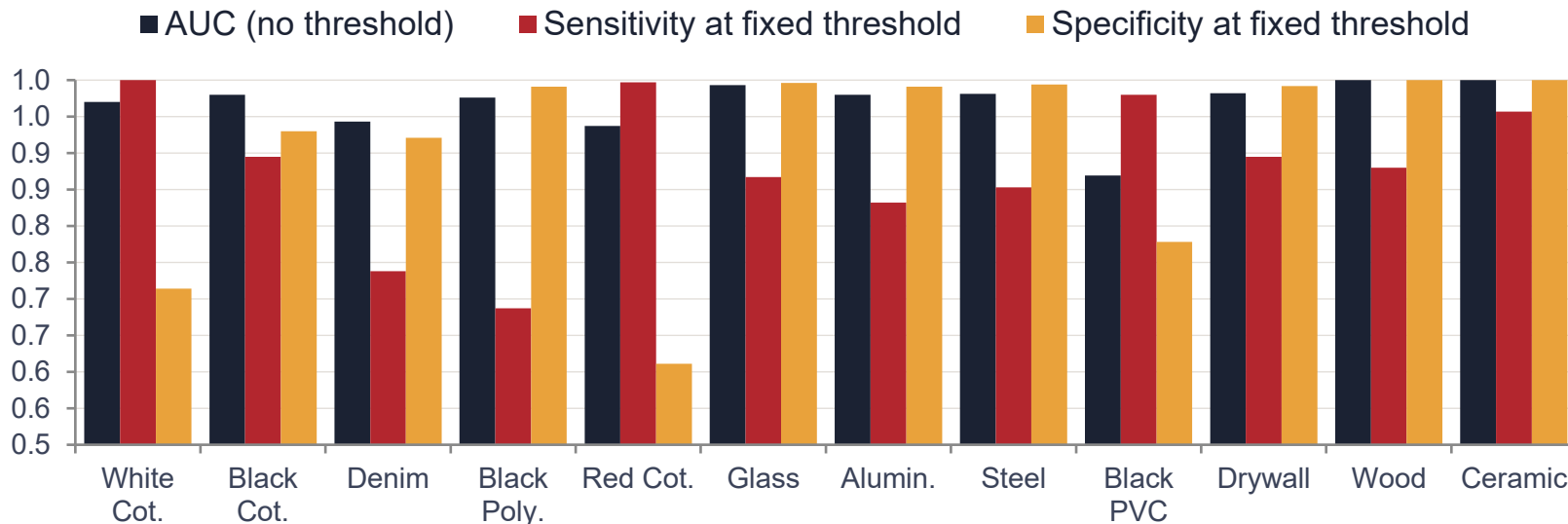
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PLS-DA classification masks



- Bright and reflective substrates: stains marked clearly with little coloured background
- SNV often fills the analysed region with a violet haze that reduces contrast
- Dark fabrics: rims, rings or isolated pixels rather than filled stains
- Even when the fixed threshold loses sensitivity, location and shape may remain recognisable for triage

A high AUC does not guarantee a working threshold



AUC ≥ 0.93 on 11 of 12 substrates, yet at the fixed threshold sensitivity or specificity falls below 0.75 on four (White Cotton, Red Cotton, Black Polyester, Denim Jeans).

The score still separates blood from background; the cut-off learned in the training session does not always fit the new image, hence the operator-adjustable threshold. Y axis starts at 0.5.



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Transfer depends on the substrate class



Model → Target	Bright	Reflective	Chromatic	Dark
Bright	0.81 / 0.92	0.97 / 0.86	0.45 / 0.83	0.94 / 0.31
Reflective	0.57 / 0.98	0.82 / 0.89	0.29 / 0.89	0.67 / 0.49
Chromatic	0.85 / 0.87	0.80 / 0.78	0.27 / 0.90	0.56 / 0.57
Dark	1.00 / 0.61	0.98 / 0.64	0.59 / 0.66	0.99 / 0.30

Each cell: mean sensitivity / specificity. Red = a value below 0.5.

Bright and reflective: reuse works. Chromatic: blood is missed. Dark: the background is marked too.

0.92

mean specificity between bright and reflective substrates (42 pairs)

0.42

mean sensitivity on chromatic and textured targets (36 pairs)

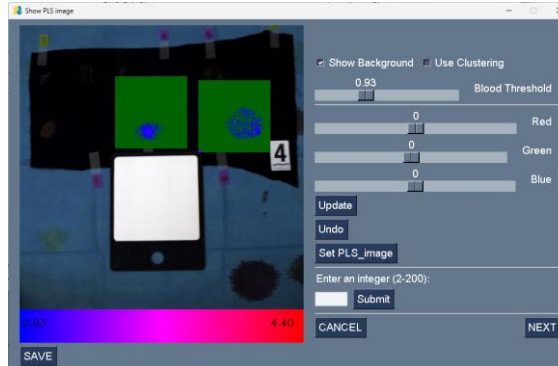
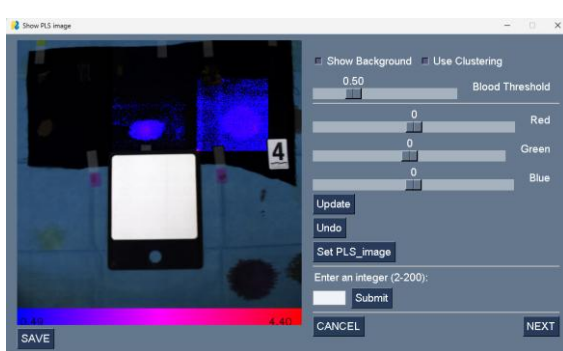
0.42

mean specificity on dark targets (36 pairs)

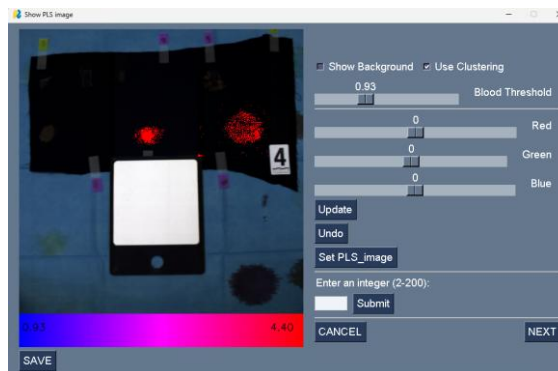


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Interactive mode: the operator sets the threshold



- Blood-threshold slider on the continuous PLS-DA score
- Show Background and optional K-Means clustering
- Guides targeted sampling without chemical treatment of the trace
- Not yet tested with operators



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Next: from blood to drug evidence



SWIR imaging

With ENEA, within NARCOSIS: the same visualize-and-classify workflow extended to the SWIR range for NPS and drug evidence. Work in progress.

Class models

To be evaluated: PLS-DA for known classes of psychoactive substances and SIMCA for samples that fit no class, linked to the naming and formulation service.

Quantification

A THC mode (PLS regression) exists in the software; it needs reference concentrations (e.g. from HPLC) before any quantitative claim.

Status: work in progress. No results on illicit drugs are shown in this talk.



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Limitations

One image per substrate per session; no stain-level confidence intervals

Only horse blood (undiluted and 1:1 diluted); no ageing, human blood or cleaned stains

A single instrument; remote consultation and DNA effects not tested

Training pixels are correlated; cross-validation is within-image and slightly optimistic

Fixed thresholds depend on the session; transfer analysis is descriptive (small classes, one deposition)

Interactive mode assessed qualitatively; no blinded operator study; no blood-free control scenes



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Take-home messages



Visualize

PCA and PLS-DA maps, with an operator-adjustable threshold, locate stealth traces on dark and reflective substrates where photography fails

Validate

First derivative had the highest external accuracy (0.905), though differences between preprocessings are small; the score stays informative, the fixed threshold transfers unreliably

Reuse with care

A threshold from another substrate fits only bright and reflective ones; chromatic and dark substrates need their own model and the operator threshold

Next: stain-level replication, operator studies, human blood and ageing, more instruments



This project has received funding from the European Union's HORIZON EUROPE innovation programme under grant agreement No. 101168195

Conclusions: are we bridging the gap?

Now...

Standardizing NPS names is a need:
new structures, precursors and
metabolites are difficult to link without
chemoinformatics

Near Future...

With ENEA, NARCOSIS is developing
HSI-SWIR tools to map the spatial
distribution of active principles in NPS
evidence (work in progress)



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innovation programme under grant agreement No. 101168195



The NARCOSIS Project is a collaboration between:



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NARCOSIS



Maj. Giuliano Iacobellis – RaCIS
Giuliano.iacobellis@carabinieri.it



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ENEA
PROJECT COORDINATOR

Backup slides



Material for questions: validation details, cross-validation curves, look-alikes, transfer analysis, limitations, naming-service internals



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Chemistry as a professional silos



IUPAC nomenclature feels artificial. Long systematic names are far from how non-specialists think about substances, so chemistry sounds like a private language rather than a practical one.

Same formula, different substance. People expect one formula to mean one thing, but isomers can share the same molecular formula and still behave very differently.

Structure matters more than intuition. A tiny change in atom arrangement can completely change properties, which is hard for non-chemists to visualize.

Reactivity is not obvious. People cannot “see” why one molecule reacts and another does not, so prediction feels abstract and rule-based.

Chemistry requires long education. Understanding names, structures, mechanisms, spectra, and conditions takes years, not minutes.

Most people must rely on authority. For non-experts, the practical way to know what a substance is often becomes “trust the label, the law, or the analyst.”

Real-world mixtures are messy. Outside the classroom, substances are rarely pure, and that makes interpretation much harder.

Analogues and derivatives create confusion. Small structural differences can produce very different legal and toxicological profiles, which is especially important for illicit drug substances.

Two-dimensional drawings hide three-dimensional behavior. Students often see flat formulas, but chemistry happens in 3D and in dynamic environments.

Chemical language is not intuitive. Common names, trivial names, trade names, and systematic names all coexist, which adds ambiguity instead of clarity.



Naming & Structure Linkage Service

«Import» brute formula (GC-MS)



Peak selection is slider-based for stability: choose a point with the slicer, then add the optional label and store the peak.

Compound Archive FT-IR / RAMAN **GC-MS** NMR HSI MS Library Search FT-IR Library Search

Upload GC-MS files

2-metilmecatnone_1MS_EI+.jdx 1.5 MB

Status

Moved to scan 130.

Loaded GC-MS files

2-metilmecatnone_1MS_EI+.jdx

Previous scan

Next scan

GC-MS slice (scan)

MS peak slicer

☐ Use label

Label text

Preview

Add MS peak

Clear peaks on current scan

Export CSV

Export TIFF

Export SVG

Chrom X min

GC-MS preview

GC-MS - 2-metilmecatnone_1MS_EI+.jdx

TIC

Retention time (min)

Intensity

m/z

Info

File 2-metilmecatnone_1MS_EI+.jdx; scans 363; current scan 130 at 6.265 min; picked peaks on this slice: 0

Picked peaks for current scan

scan	mz	intensity	label
------	----	-----------	-------

Download report



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Technical Recap of NSS:

Chemoinformatic in practice



1. RapidFuzz Engine – Textual String & Slang Normalization

- **Primary Role:** Normalizes noisy operational LIMS inputs, regional street slang (e.g., "pink cocaine"), trade names, typos, and long IUPAC strings.
- **Core Algorithms:**
 - WRatio:** Merges Levenshtein distance, TokenSort, and TokenSet to handle word order permutations and token overlap.
 - WSubstring:** Detects specific chemical acronyms or partial strings embedded within longer narrative descriptions.
- **Deployment:** Serves as a Python **FastAPI REST microservice** (/v1/normalize) connected to the local NPS Registry (*now csv based to be accessible to practitioners for revision*).

2. RDKit Engine – Structural Intelligence & Validation

- **Primary Role:** Evaluates molecular chemical structures (SMILES, Mol blocks) rather than text strings.
- **2048-Bit Fingerprinting & Tanimoto Math:** Converts 2D structures into 2048-bit RDK fingerprints and quantifies molecular overlap:
$$\text{Tanimoto}(A, B) = \frac{|A \cap B|}{|A \cup B|}$$
- **Structure Classification:** Resolves layered InChIKeys (XXXXYY-ZZZZ-A) and *in future will apply* SMARTS reaction rules to discover **Isomers**, **Precursors**, **Metabolites**, and **Analogues**.



Trend Analysis Suite: Collection based analysis



NARCOSIS Non-Targeted forensic multidisciplinary platform for investigation of drug-related fatalities

Logged in as: Administrator (Logout)

Illicit Drug Trends

- Upload CSV
- Import from NARCOSIS
- NARCOSIS data
- Plot
- Table View**
- Illicit Drug Trends
- NPS Trends
- Pills Trend
- Potency corr
- Recap Dashboard

View & Combine Collected Files

Collected Files

Select file to preview:
monthly_2023-01

Select files to delete:

- monthly_2023-01
- monthly_2023-02
- monthly_2023-03
- monthly_2023-04
- monthly_2023-05
- monthly_2023-06
- monthly_2023-07
- monthly_2023-08

Concatenate All Files
Combine all collected files into a single dataset for trend analysis.
[Concatenate All Files](#)

✓ Concatenated dataset ready: 24361 rows x 14 columns

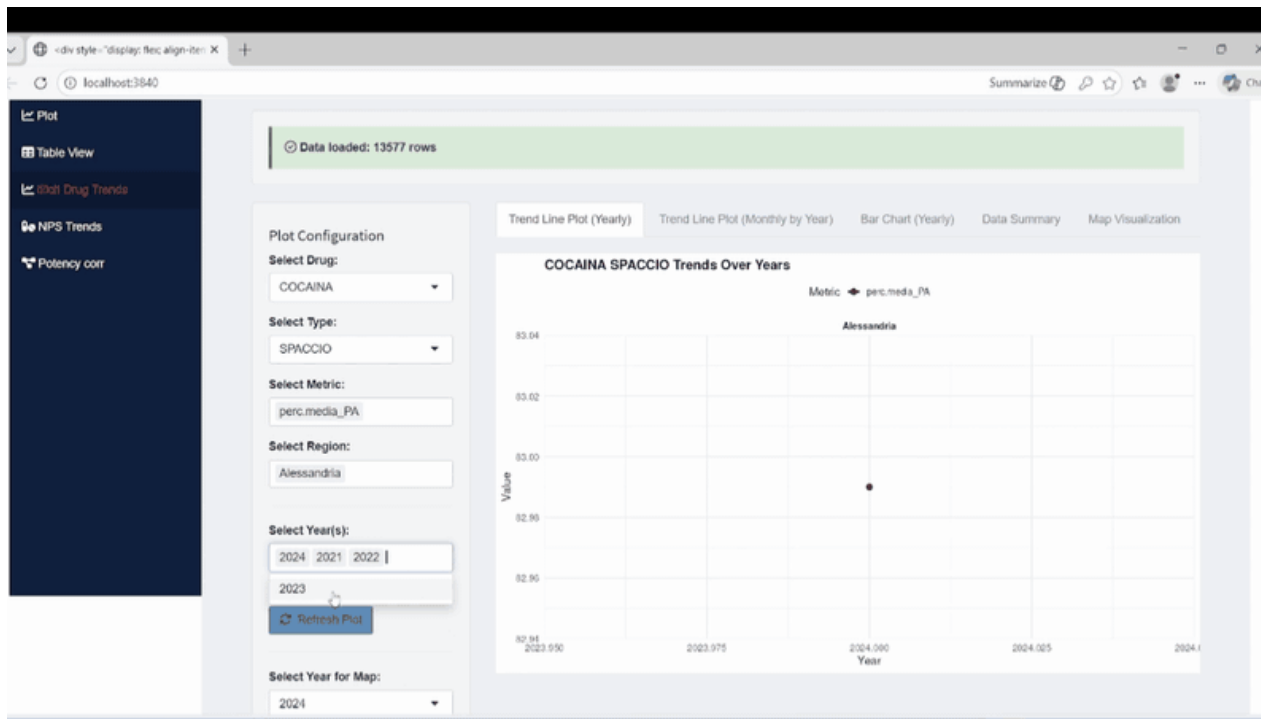
Show 15 entries

FileSource	gruppi_reg	metric	value	formatted_row	Date	Period	Drug	Type	Region	Metric
monthly_2023-01	Centro	perc.media_PA	11.58	2026/09/21 2023-01 MARIJUANA SPACCIO Centro perc.media_PA 11.58	2026/09/21	2023-01	MARIJUANA	SPACCIO	Centro	perc.med



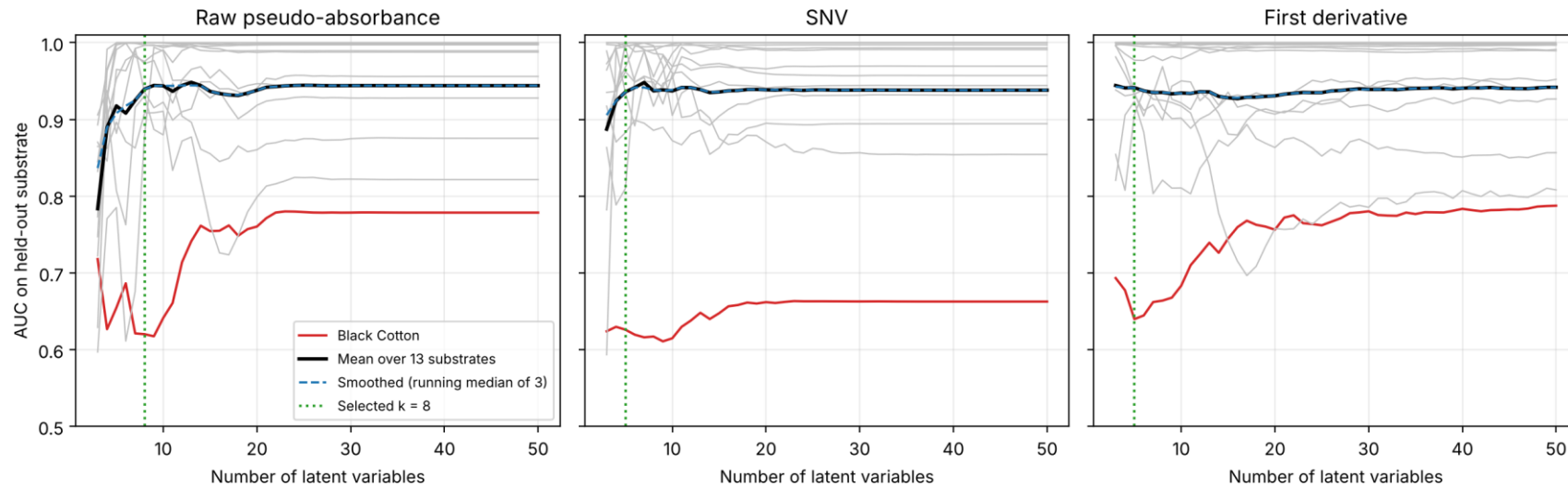
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Trend Analysis Suite: Temporal evolution



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Latent variables chosen across substrates

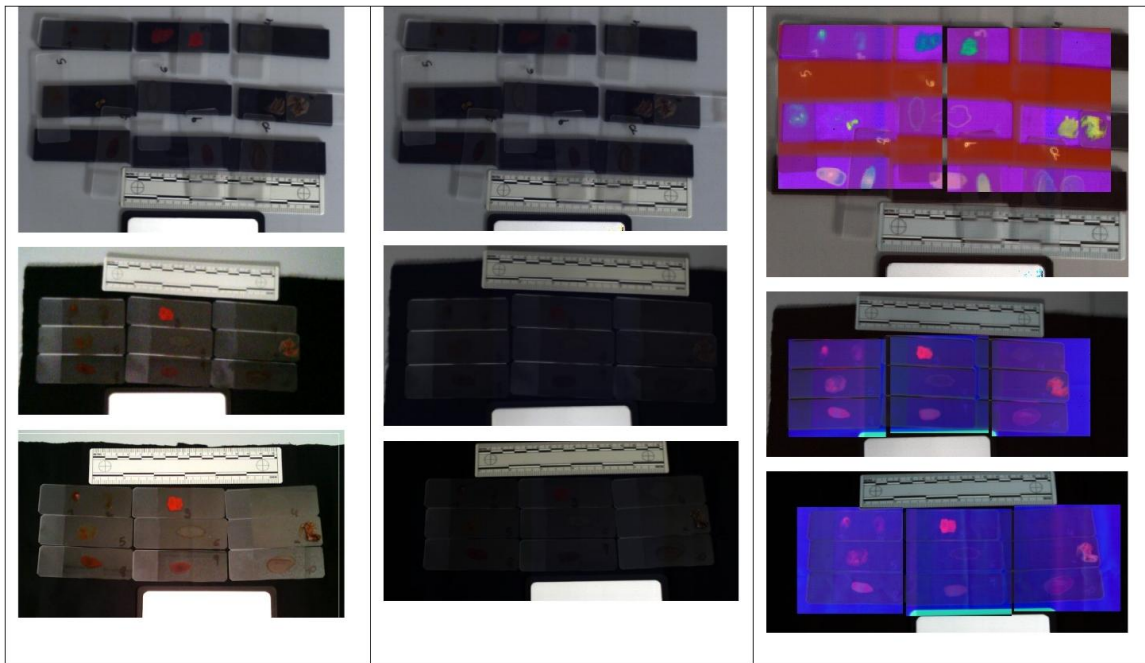


- One k per preprocessing: 8 (raw), 5 (SNV), 5 (first derivative)
- Held-out AUC plateaus: 0.927–0.944 for first derivative over 3–50 LVs, so the exact k is not critical
- Black Cotton stays at AUC 0.64 whatever the setting (red)



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Porous dark fabrics limit visibility



- Blood deposited on glass placed over the dark substrates
- Diffusion into the fabric is prevented and contrast rises markedly
- So penetration, not missing spectral information, limits dark porous fabrics



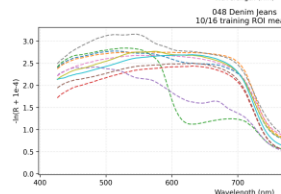
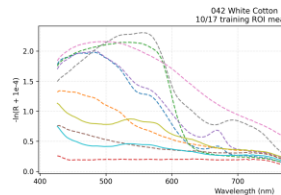
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Preprocessing changes the spectra

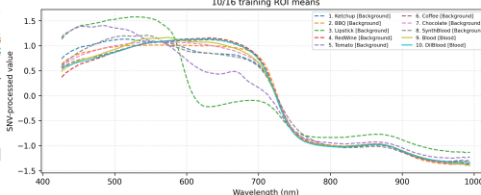
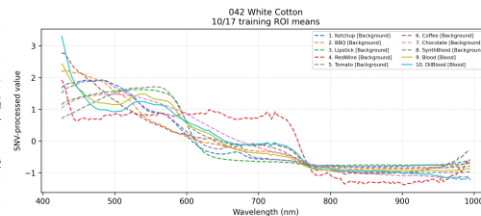
Training spectra by substrate - separate ROI means
Log-transformed spectra: $\ln(R + 1e-4)$
Solid: blood-labeled ROI; dashed: background-labeled ROI

Training spectra by substrate - separate ROI means
Log-transformed spectra followed by ChSI SNV
Solid: blood-labeled ROI; dashed: background-labeled ROI

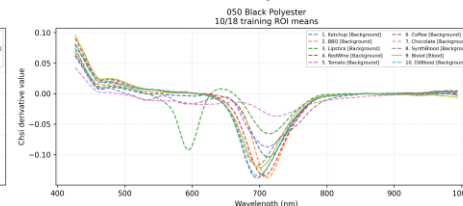
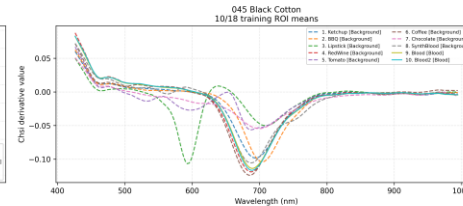
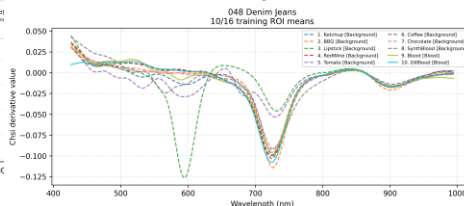
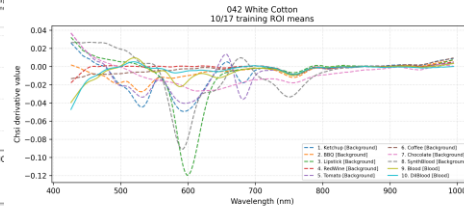
Training spectra by substrate - separate ROI means
Log-transformed spectra followed by ChSI derivative
Solid: blood-labeled ROI; dashed: background-labeled ROI



None (raw pseu)



SNV



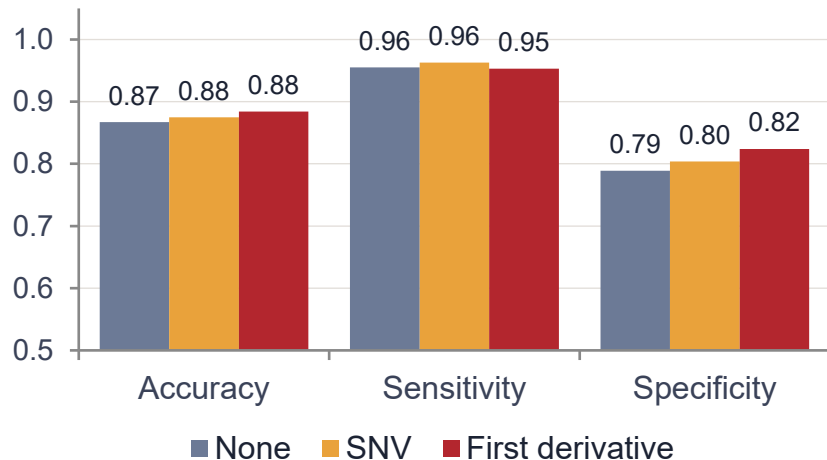
First derivative



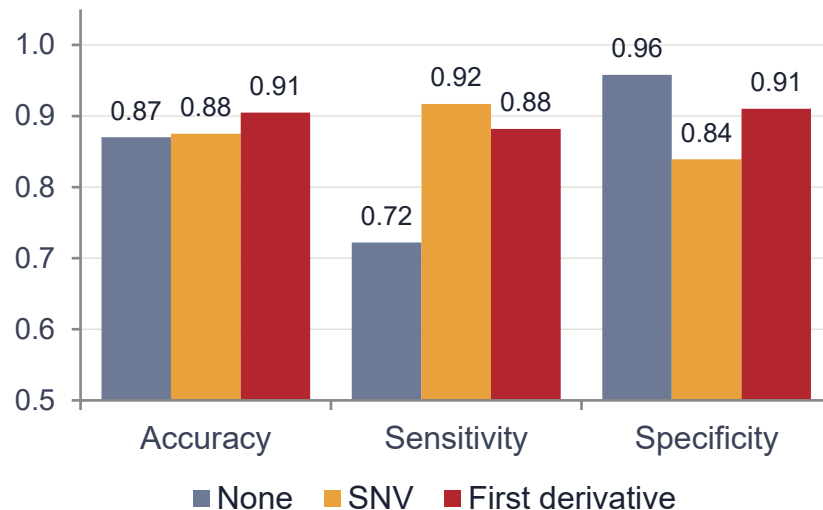
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Cross-validation versus external session

ROI-grouped cross-validation
(TRACCE)



External session (TRACCE_BIS)



Cross-validation is descriptive (within-image). The external session is the stronger test: first derivative has the highest mean accuracy (0.905) and the most balanced sensitivity and specificity, but differences between preprocessings are small relative to substrate effects.



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False positives on look-alike traces

Look-alikes: ketchup, BBQ sauce, lipstick, red wine, tomato sauce, coffee, chocolate, synthetic blood

7 of 96

trace-image combinations with a false-positive rate of 0.5 or more (first derivative)

13 of 96

with SNV

3 of 96

with raw pseudo-absorbance

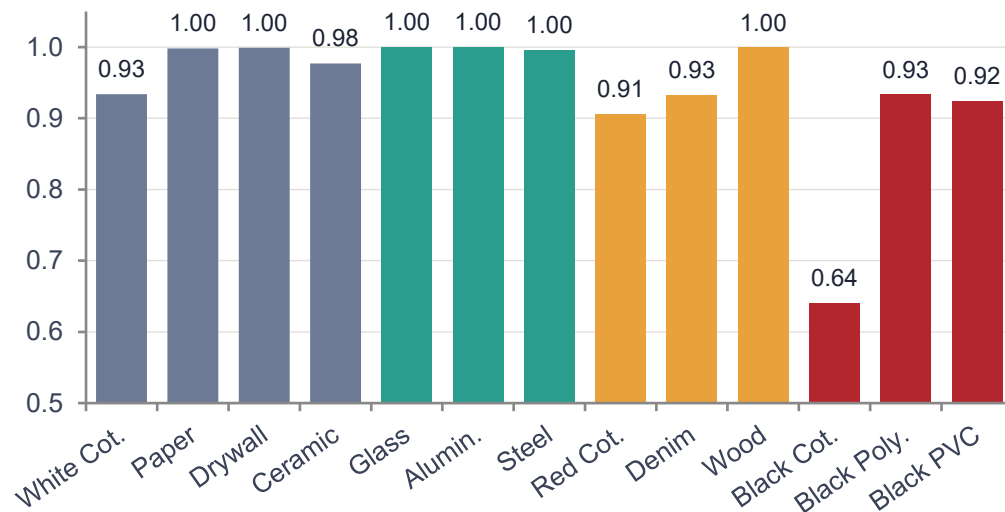
- No look-alike called blood on White Cotton and Ceramic with SNV, but the low rates there depended on the preprocessing
- Dark and coloured substrates carry most of the false positives, which is why the operator can adjust the threshold



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Two questions about using a model elsewhere

1 Does the score still separate blood?



Held-out AUC, first derivative (bars: bright, reflective, chromatic, dark). Model trained on the other 12 substrates.

2 Does the threshold transfer?

22 of 156

single-substrate models reach 0.9 on both sensitivity and specificity on another substrate; 21 of those 22 have a bright or reflective target

So the score ranks blood correctly almost everywhere, but a fixed threshold from another substrate usually does not fit.

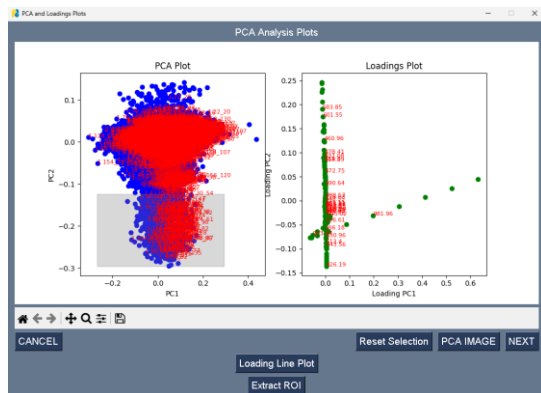
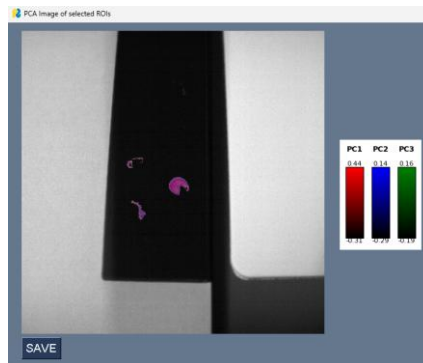
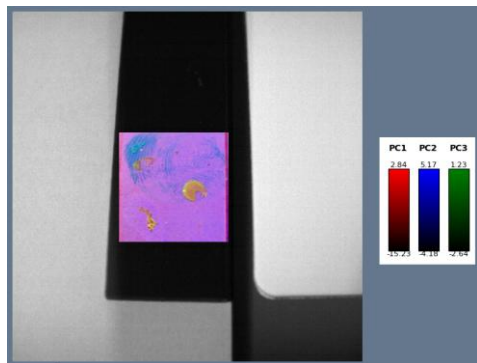


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PCA selection and remote collaboration



- PCA composite of an operator-selected region, with interactive selection in the score plot
- Records can be shared with remote colleagues through the RISEN portal
- Latency and field network performance were not measured



RISEN portal interface showing a case summary and a table of measurements.

Case Summary:

- ID: 030a03-3764-46b-8975-10a102716a01
- Category: N/A
- Sensor: SPECIM IQ
- Case: Test case 2
- Status: Pending
- Created at: Dec. 5, 2023, 4:10 p.m.
- Modified at: Dec. 5, 2023, 4:10 p.m.

Measurements Table:

Label	Date/Time	Type	Sensor	Status
030a03-3764-46b-8975-10a102716a01	Dec. 5, 2023, 10:25 a.m.	2D Measurement	SPECIM IQ	Pending
030a03-3764-46b-8975-10a102716a01	Dec. 5, 2023, 10:25 a.m.	Far 2 Spectra (CSI)	SPECIM IQ	Pending
030a03-3764-46b-8975-10a102716a01	Dec. 5, 2023, 10:25 a.m.	ROI (CSI)	SPECIM IQ	Pending
030a03-3764-46b-8975-10a102716a01	Dec. 5, 2023, 10:25 a.m.	Selected ROI Picture	SPECIM IQ	Pending
030a03-3764-46b-8975-10a102716a01	Dec. 5, 2023, 10:25 a.m.	Far 2 Spectra (CSI)	SPECIM IQ	Pending
030a03-3764-46b-8975-10a102716a01	Dec. 5, 2023, 10:25 a.m.	ROI Spectra (CSI)	SPECIM IQ	Pending



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What decides whether a model can be reused



Bright and reflective

Works

Threshold transfers: mean specificity 0.92; 14 of 42 pairs reach 0.9 on both metrics



Chromatic and textured

Score still ranks blood (Wood AUC 0.999) but it falls below the threshold: mean sensitivity 0.42



Dark

Background marked too

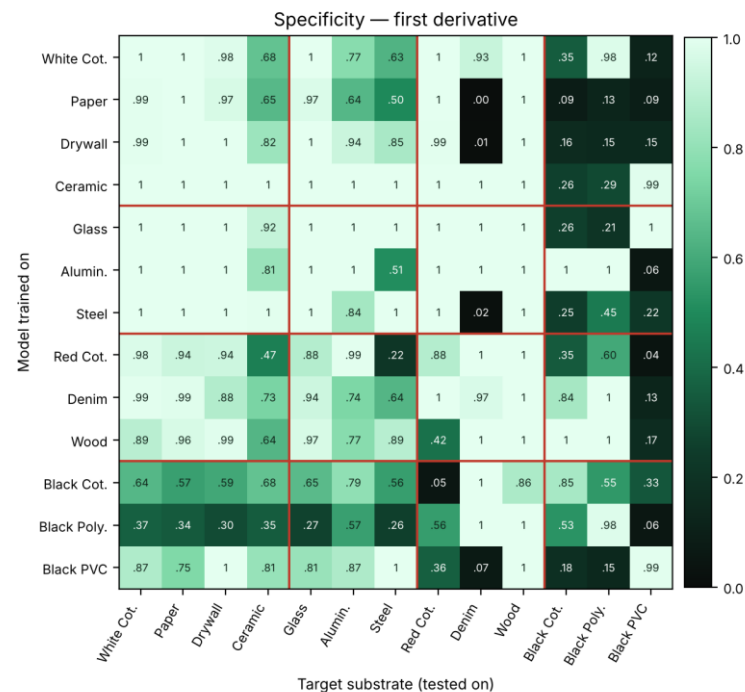
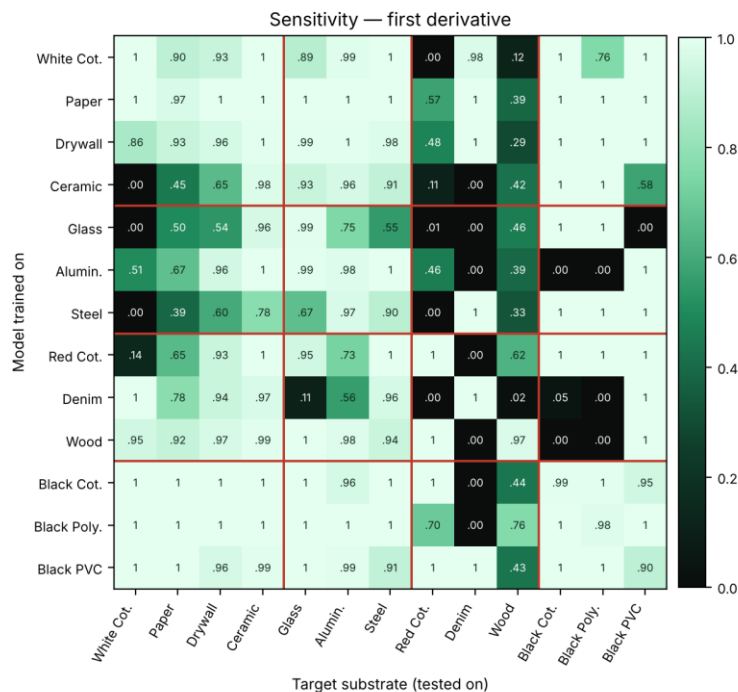
Blood detected but so is the background: mean specificity 0.42 (score AUC 0.92–0.93 on PVC, Polyester; 0.64 on Black Cotton)

The score separates blood almost everywhere; what changes between substrate classes is whether a threshold fitted elsewhere still fits.



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Appendix: threshold transfer between substrates



How to read: each row is a model trained on one substrate, each column the substrate it is tested on; dark = 0, light green = 1. The diagonal is the model on its own training pairs (in this case) Black: bright reflective, chromatic, dark. The 156 off-diagonal pairs have 0.920 sensitivity and 0.73 specificity.



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