

Real time qualification and quantification of illicit drugs using Near-infrared spectroscopy connected with mobile phone application.

Cours : Introduction to machine learning for bioengineers

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Ecole des sciences criminelles

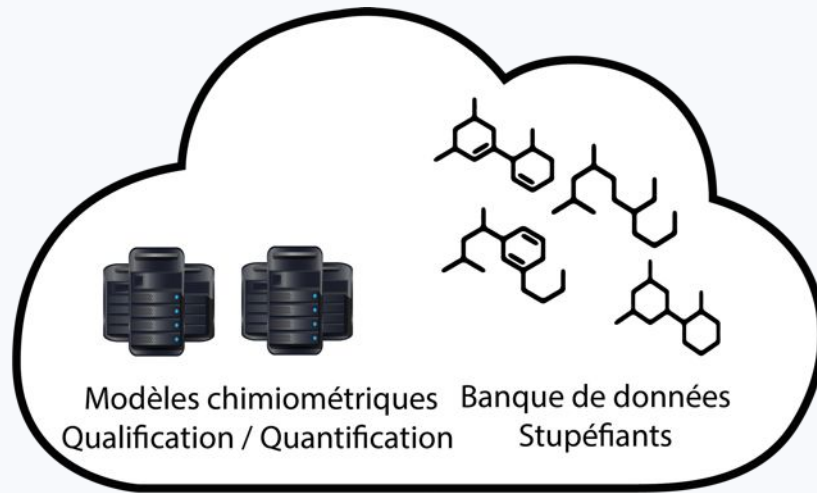


Real time monitoring of substance through Decentralization of forensic capabilities

- Real time results
- Early warning
- Early response

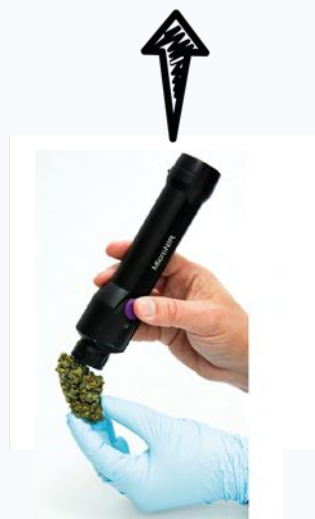


NIRLAB Architecture



NIRLAB Cloud

- Stockage des résultats
- Traitement des analyses par des modèles chimiométriques



MICRONIR



NIRLAB Mobile App

- Reçoit les résultats des scan
- Envoie les données sur le cloud
- Affichage des résultats



NIRLAB Desktop App

- Monitoring des résultats
- Analyses spatiales et temporelles
- Détection Hotspot
- Détection nouveau phénomène



Analyse en 5 secondes

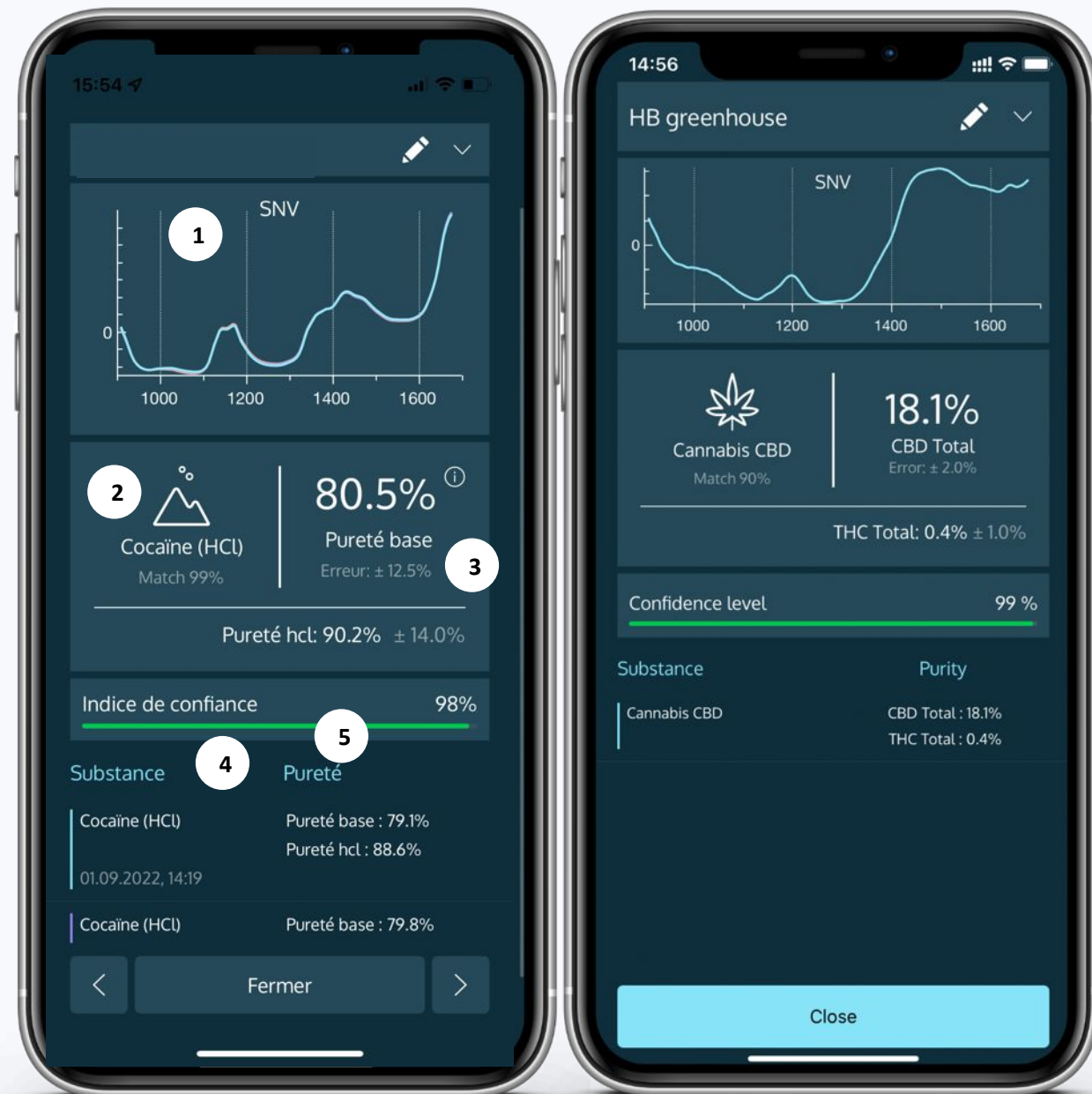


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NIRLAB – Mobile App

Mobile app shows:

1. NIR spectra
2. Identification of the substance
3. Quantification information
4. Cutting agent (if available)
5. Confidence level



Advantages of NIRLAB

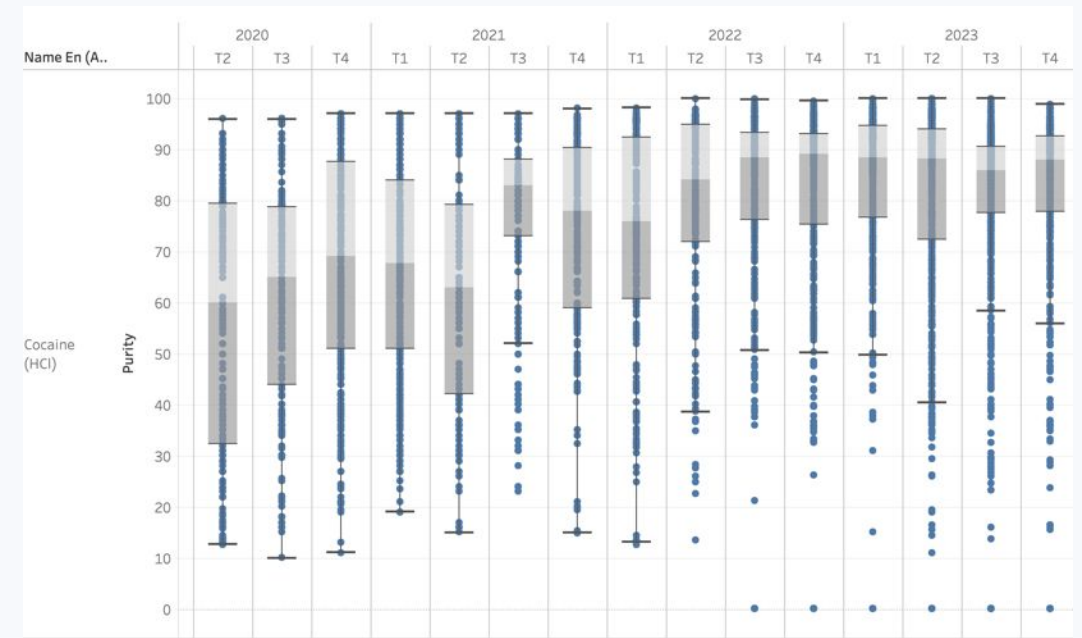
- > No sample preparation
- > No chemicals required
- > Non-destructive
- > Real-time analysis
- > Ultra-potable
- > Cloud-oriented
- > User-adaptable (mobile app and website)
- > Adaptable to new substances (NPS)

Illicit drugs

Illicit drugs	Qualitative	Quantitative
Cannabis	CBD-type vs THC-Type	yes
Hashish / Resin	yes	yes
Marijuana	yes	yes
Cocaine, Crack	yes	yes
Heroin	yes	yes
MDMA / Ecstasies	yes	yes
Methamphetamine	yes	yes
Amphetamines	yes	yes
Ketamine	yes	yes
NPS - choix	yes	non
More than 120 standards of different compounds in the DB		

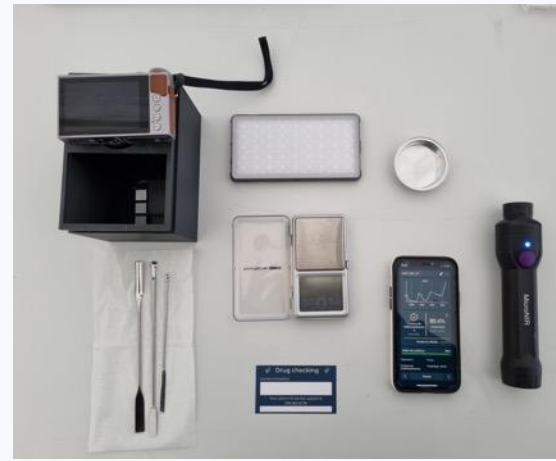
Law enforcement

- Police
- Customs
 - Real time
 - Qualification
 - Quantification
- Intelligence (live monitoring)
- Before only 5% analyses now 95%



Drug checking

- Permanence
- Music festival
- Injection rooms
 - Real time
 - Qualification
 - Quantification
 - Intelligence (live monitoring)



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Fields of application

Counterfeit medicines

Doping product

Illicit drugs



Fungus Detection



Pharmaceutical Drugs Identification



Doping Product



Narcotics Identification



Plastic Identification for Recycling



Mineral Identification for Field Exploration



Food Quality Inspection



Moisture in Materials



Bacteria Detection



Coating Reflectance



Paint Pigment Testing



Soil Monitoring



Textile Fabrics Identification



Agricultural Plant Health Monitoring



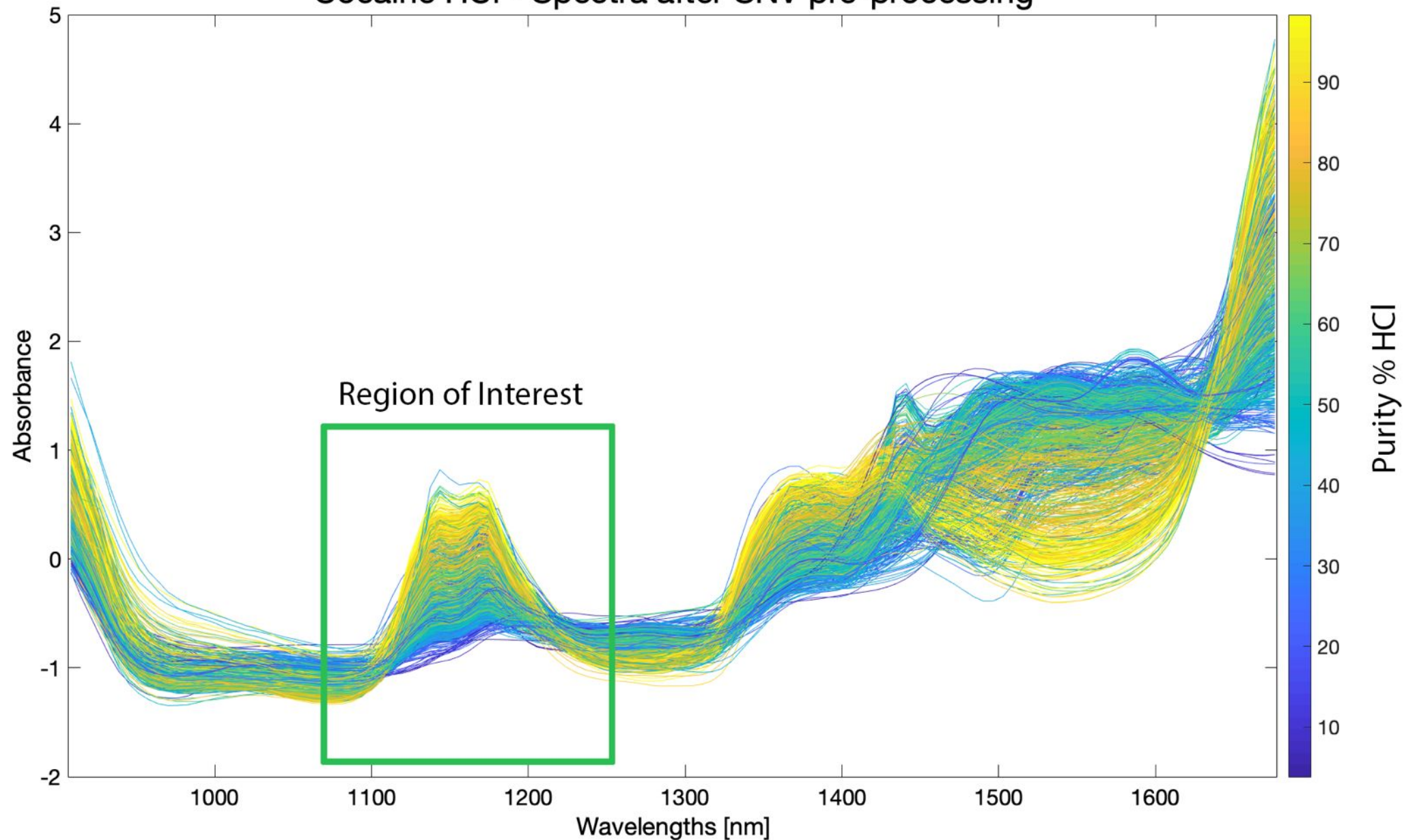
Explosive

Cannabis quality control

Explosif

The NIR spectra

Cocaine HCl - Spectra after SNV pre-processing



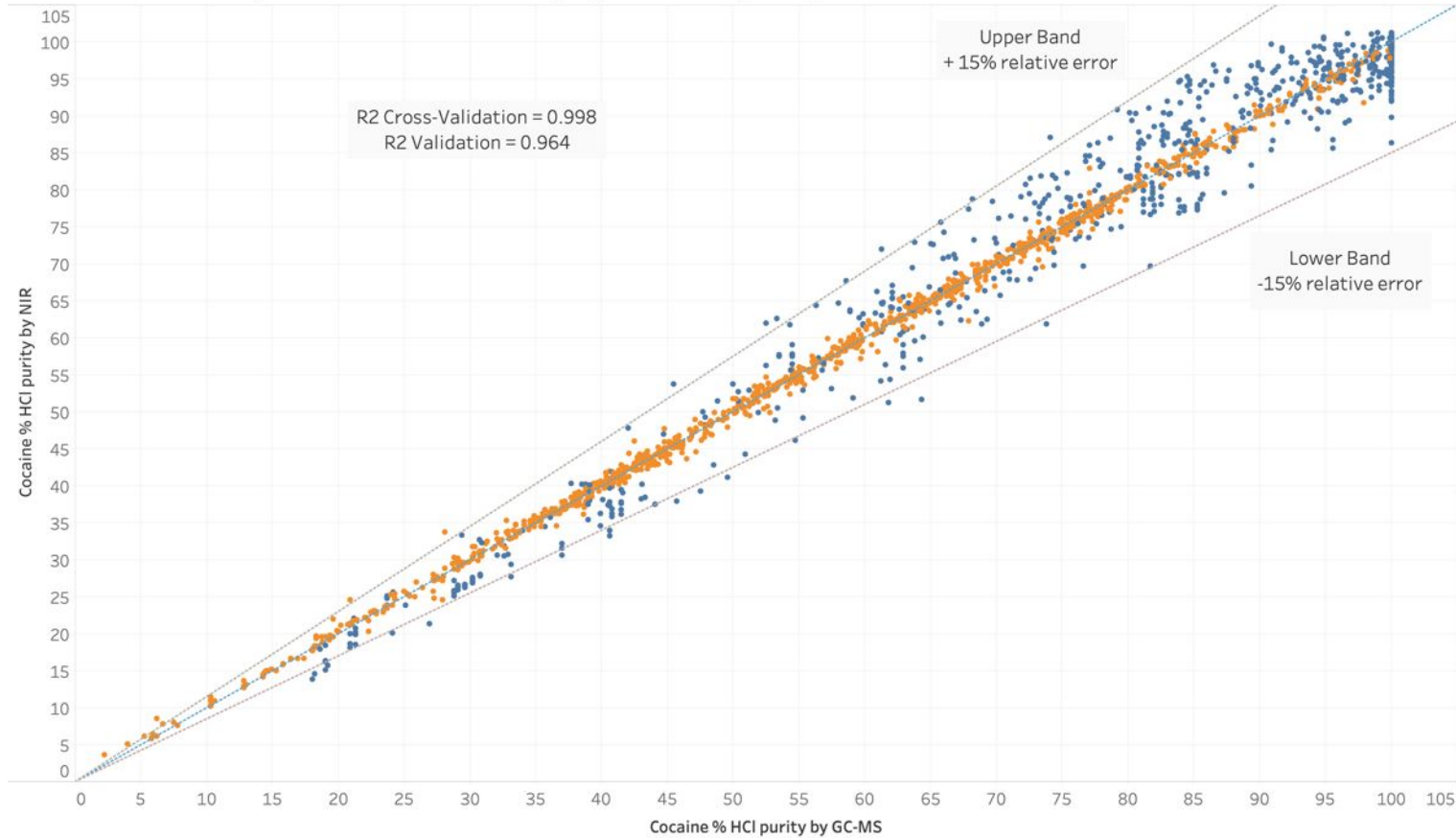
Qualitative performance

Confusion matrix of cocaine predictions for 2047 specimens (calibration, validation and external validation) of cocaine. P=Positive, N=Negative, TP=True Positive, FP=False Positive, TN=True negative, FN=False negative.

Cocaine (2047 samples)		microNIR		
Non-cocaine (182 samples)		P = 2035	N = 194	
GC-MS	P = 2047	TP = 2035	FN = 12	Sensitivity = 0.994 (TP/P)  ✓
	N = 182	FP = 0	TN = 182	Selectivity = 1 (TN/N)  ✓

Quantitative performance

Cocaine Validation Set - Quantitative model - Predicted (NIR) vs Reference (GC-MS)



Substance	Total
Cocaine	1437

↓

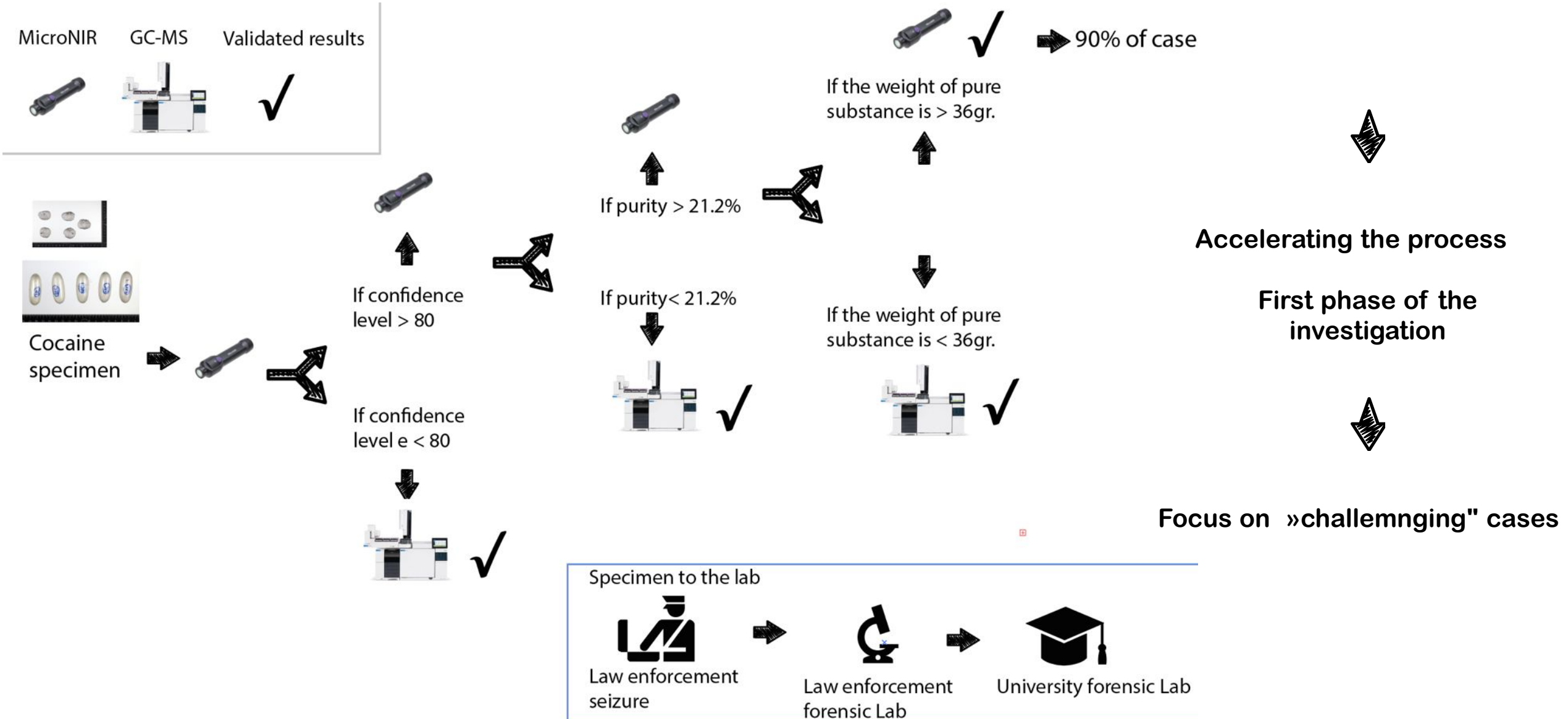
Calibration	Validation
966	471

↓

Purity Range
5% - 100%

Cocaine MicroNIR method		Cocaine ISO 17025 validated GC-MS method	
Concentration (%)	Relative Expanded Uncertainty (%)	Concentration (%)	Relative Expanded Uncertainty (%)
$21.2 \leq C < 40.5$	15.5	$1.15 \leq C < 5.5$	17.0
$40.5 \leq C < 81.6$	12.5	$5.5 \leq C < 69.8$	10.0
$81.6 \leq C \leq 98.5$	7.7	$69.8 \leq C < 87.3$	13.0

Legal use (ISO 17025)



Legal use - Control of the spectra

Visualize

Refresh

Plots:

☒ PCA ☒ Spectra

☒ Auto-update PCA

Preprocessing

2D5 + SNV | 2nd Derivative (order: 2, window: 5 pt, tails: 0)

Substances

Color by

Purity

Mark by

calibration status

Basic Tools

Refresh

Kennard Stone

66 %

☒ Show Plots

Classification

Regression

PLS

N components

6

Machine Learning

Refresh

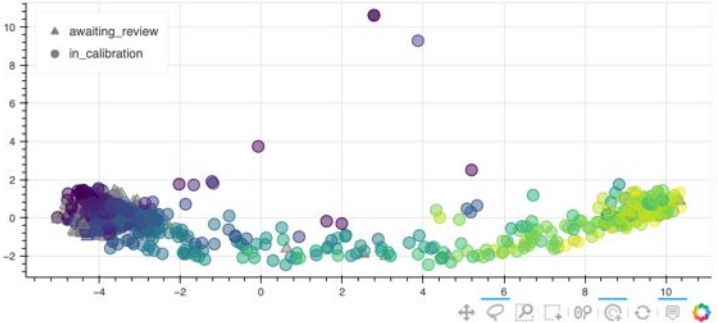
☒ Production ☐ AutoML

Preprocessing

2nd Derivative (order: 2, window: 5 pt, tails: 0)

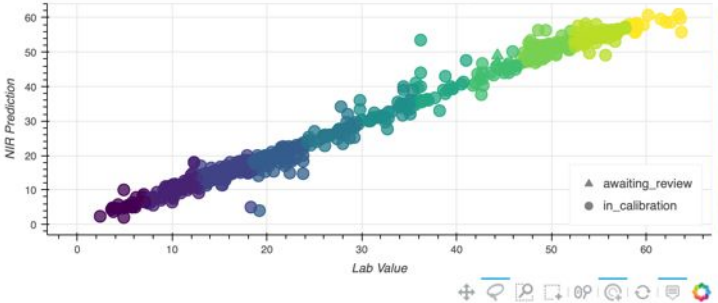
▲ awaiting_review

● in_calibration



Search

Production Results for model hero_base

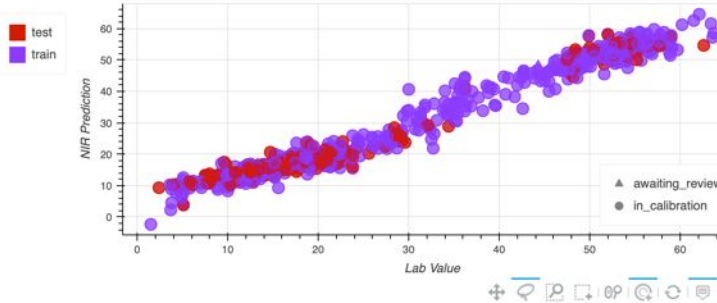


882 selected samples

test

train

PLS Regression Model



Bulk Actions

Date	Name	Substance	Confidence	Added by
08/06/21 11:26	ctrl-her-01-ref	Heroin (base) Purity Base: 13% (-2.3%) caffeine Estimate +	99 %	Labo ESC (ESC-Stups)
24/05/21 15:20	ctrl-her-02-ref	Heroin (base) Purity Base: 49% (10.6%)	99 %	Labo ESC (ESC-Stups)

total: 5726
samples selected: 882
samples without spectrum: 0 update

Date from

21 / 10 / 2021

☐ Only Samples with purity

Calibration Status

Awaiting review (72)
In calibration (810)
Excluded
Outlier

Substance Forms

Homogenized Powder
Non homogenized powder
Finger
Crystals
Brick
Pill
Pellet
Bud
Plant
Hashish
Other
Unspecified (882)

Measure types

Plastic Bag
rigid plastic
Transparent glass
Direct contact (882)
Unspecified



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