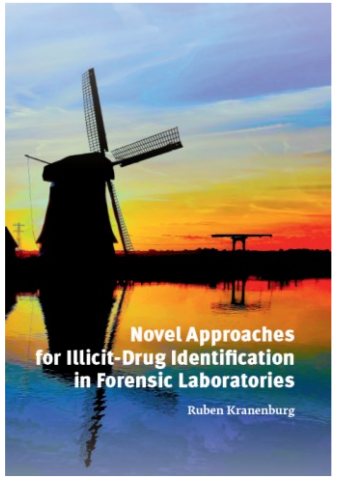
How can NIR spectroscopy contribute to rapid, on-scene and court-admissible drug identification?

Ruben Kranenburg

Introduction

Dr. Ruben Kranenburg
lead specialist drug analysis, Dutch Police
scientist, forensic analytical chemisty, University of Amsterdam

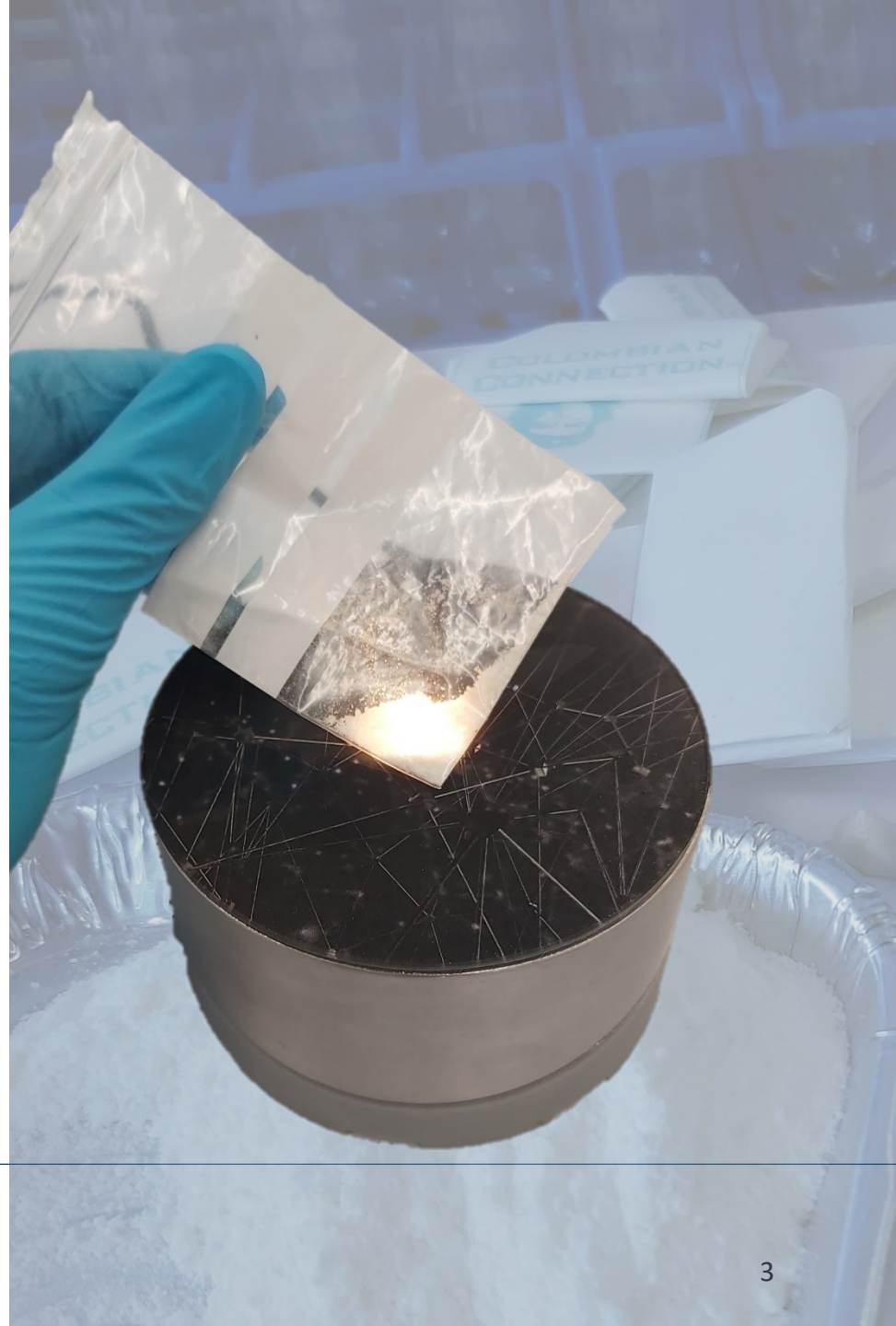


POLITIE

UNIVERSITY OF AMSTERDAM

Outline

- Illicit-drug market in The Netherlands
- Forensic laboratory testing
- Portable Near-Infrared analysis
  1. NIR sensors
  2. Sensitivity & Specificity for drugs
- Conclusions
- Future Outlook: towards implementation



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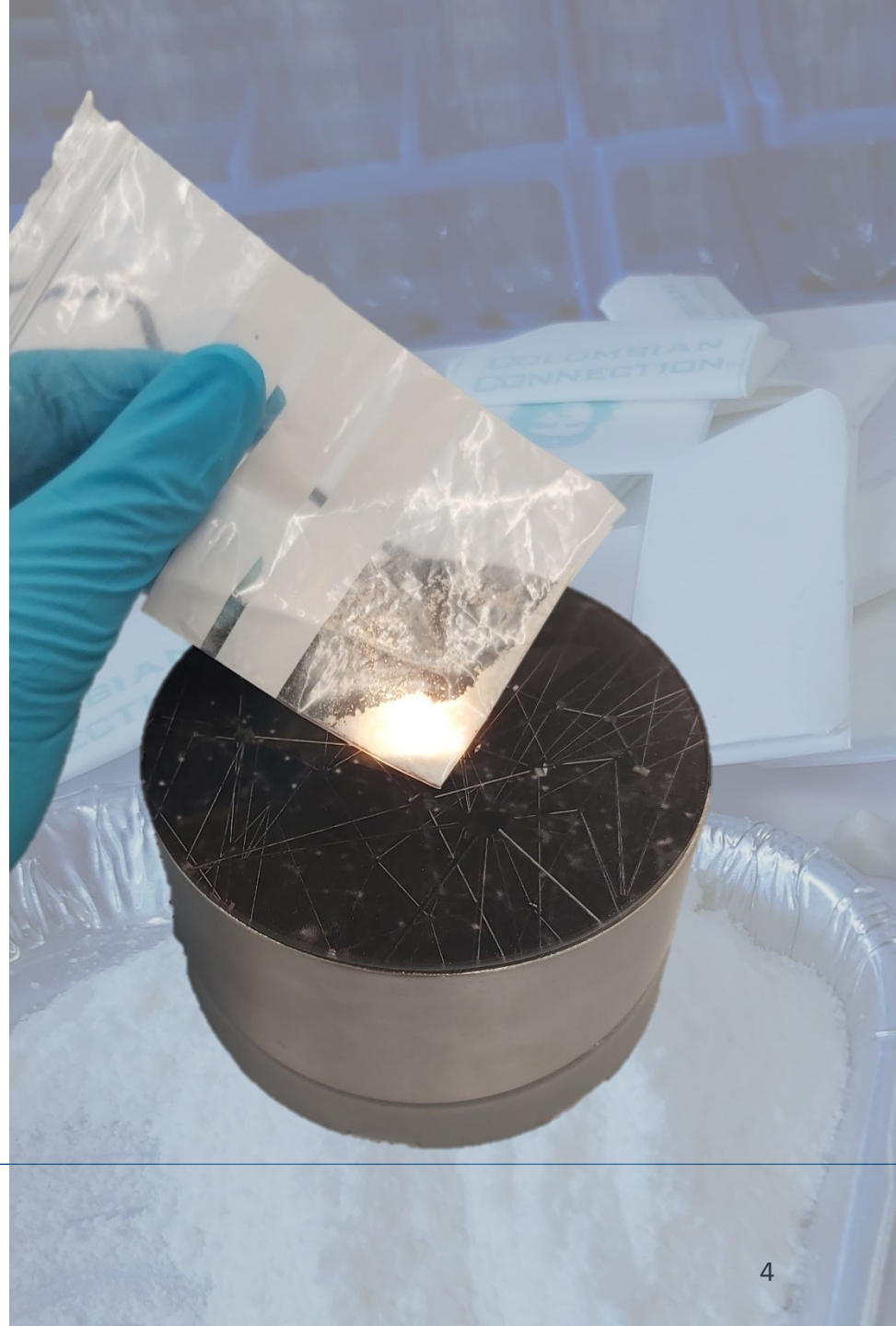
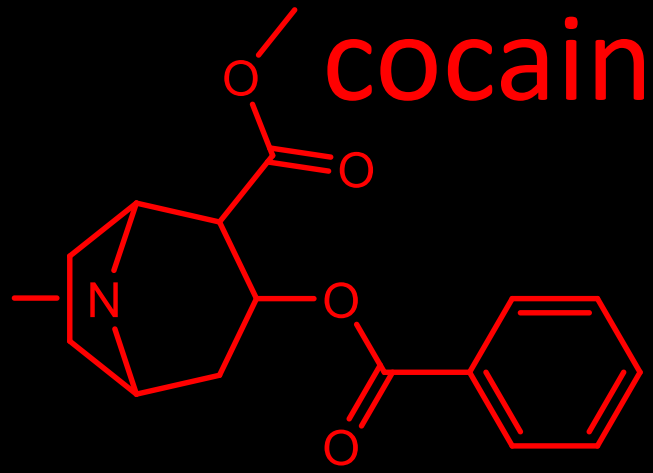
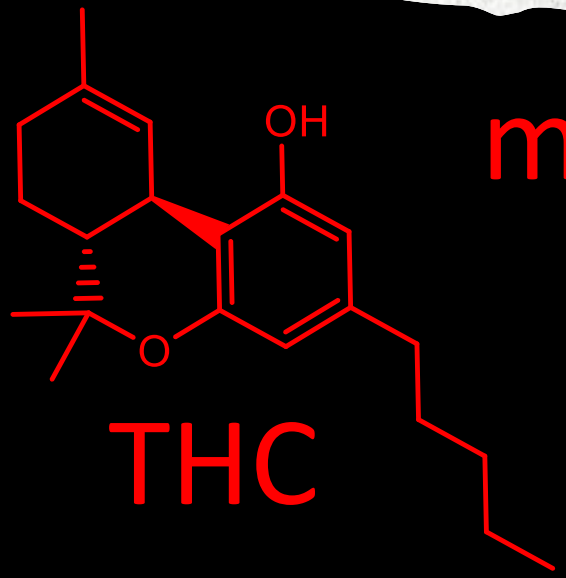


cocaine

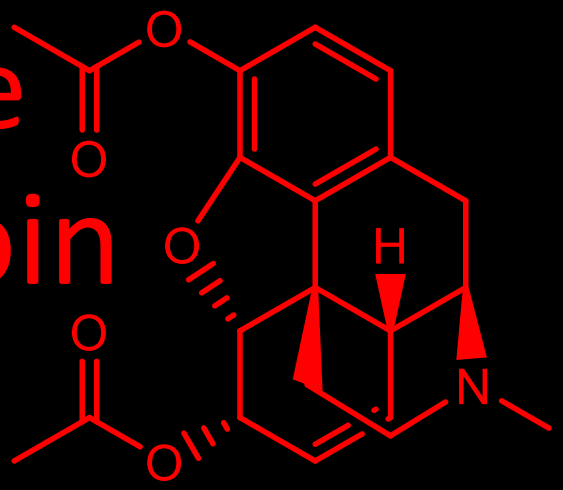




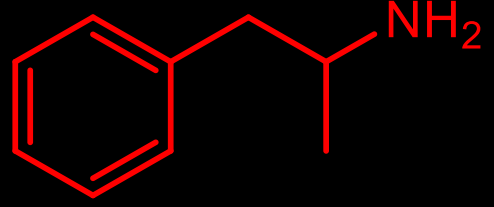
THC

morphine

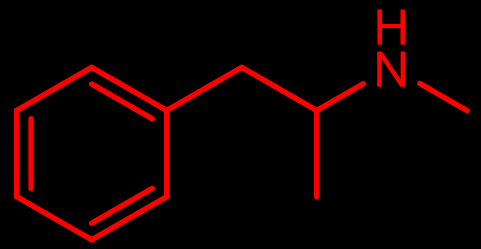
heroin



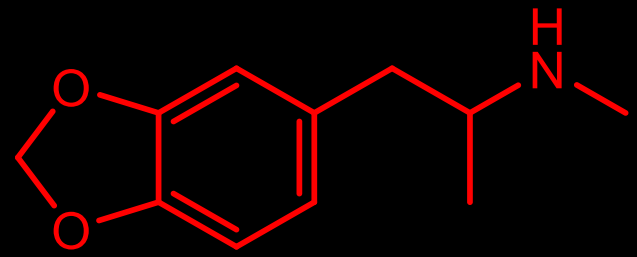
‘Traditional’ drug products



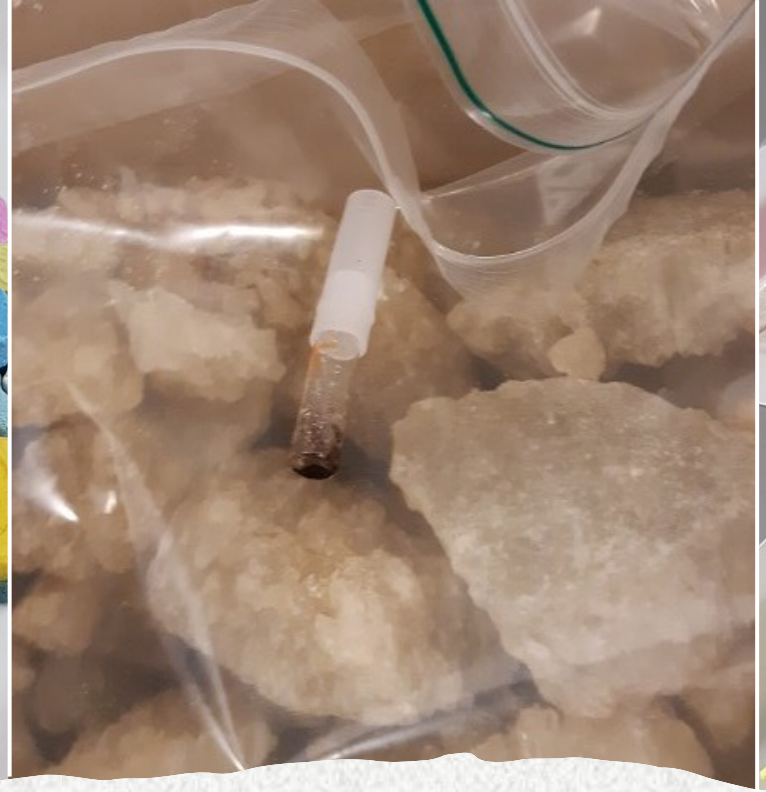
amphetamine



methamphetamine



MDMA



Synthetic drugs

Annual workload

~ 25.000 samples

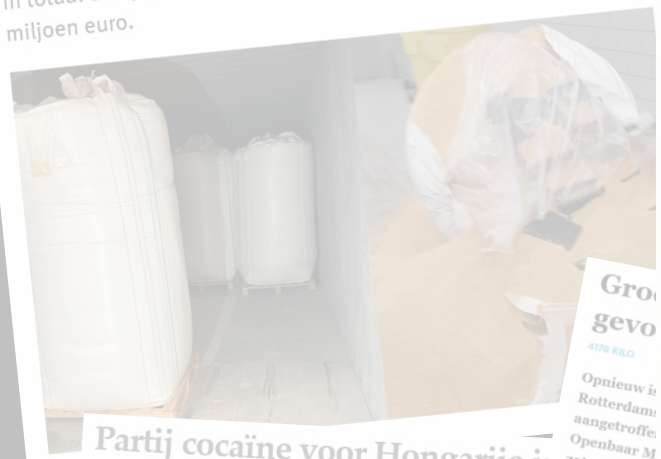
~ 5.000 samples

Amsterdam

Douane onderschept enorme partij cocaïne: 4178 kilo

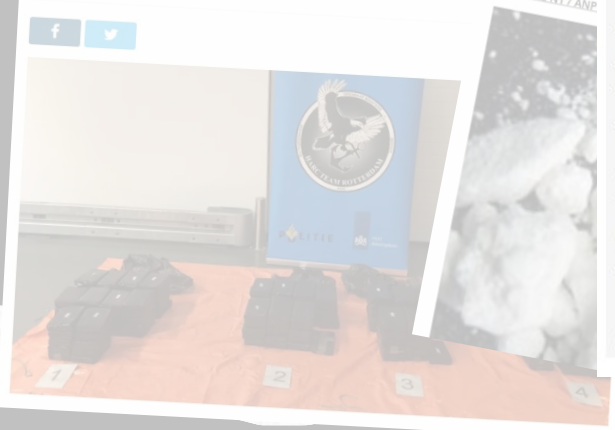
Nieuwsbericht | 31-10-2021 | 12:30

Tijdens een controle in de Rotterdamse haven heeft de Douane gisteravond een enorme hoeveelheid cocaïne onderschept. Het gaa in totaal om 4178 kilo cocaïne met een straatwaarde van ruim 313 miljoen euro.



Partij cocaïne voor Hongarije i Rotterdam onderschept

10 juni 2021



Drugs

March 2023

The Guardian

Cocaine smuggling and production at record high since pandemic retreat

New UN report says there has been a 35% spike in 2020-21 in the production of coca, the drug's base ingredient

16 Mar 2023

3000 kilo cocaïne onderschept in Rotterdam, straatwaarde 225 miljoen

16 juli 2021 10:35

Aangepast: 16 juli 2021 11:19

n 4.178 kilo en 313

controle in de Rotterdamse haven, een enorme hoeveelheid cocaïne t een straatwaarde van ruim 313 miljoen euro', zo meldt het Openbaar

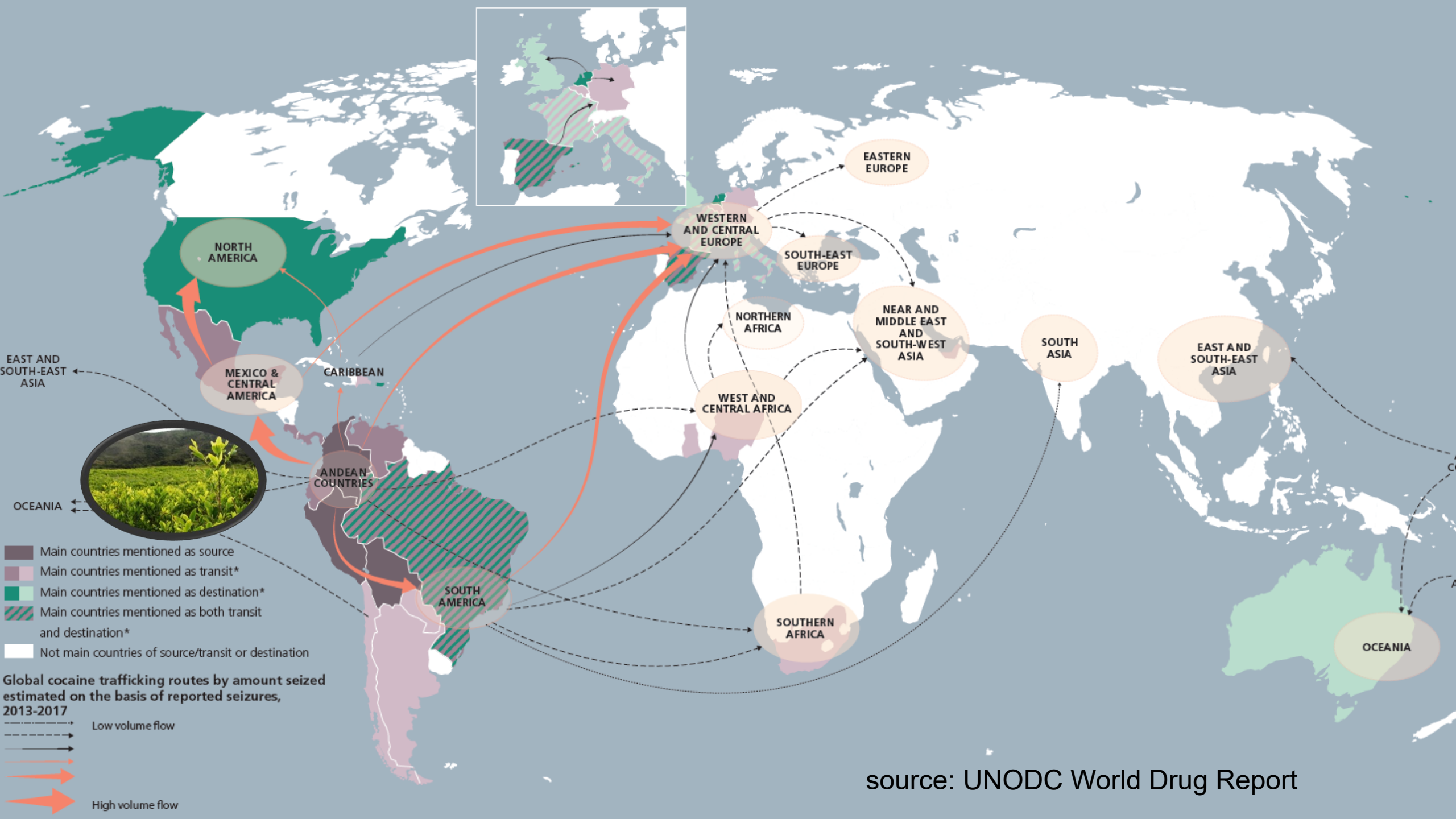
100 kilo coke onderschept op Schiphol

het CargoHarc-team van Schiphol heeft deze maand een rtij cocaïne uit Mexico onderschept. De drugs hadden straatwaarde van 5 miljoen euro.

'arool 20 oktober 2021, 17:18

BEELD ANP XTRA

The increasing amounts of drugs



source: UNODC World Drug Report

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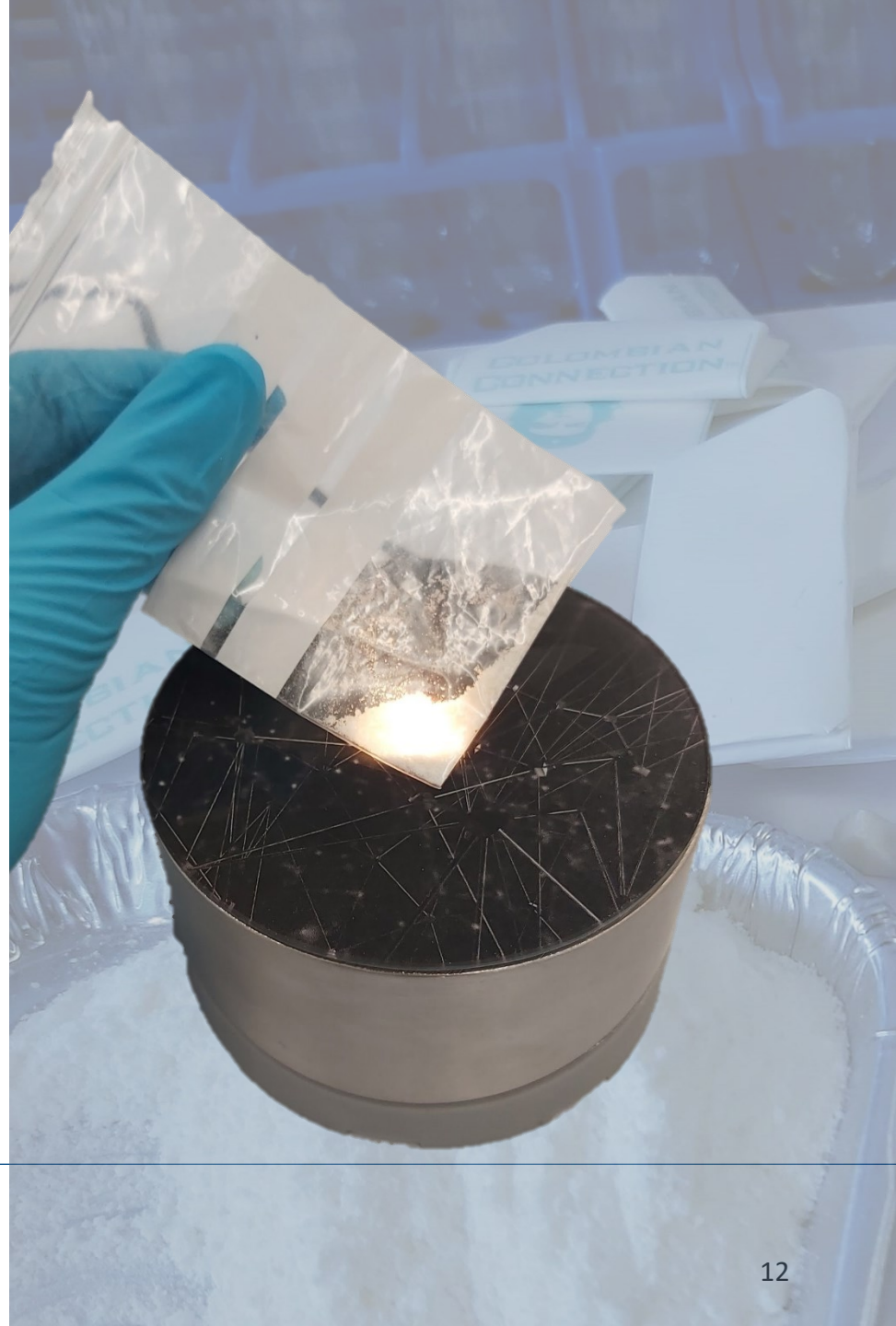


1916

Co van Ledden Hulsebosch

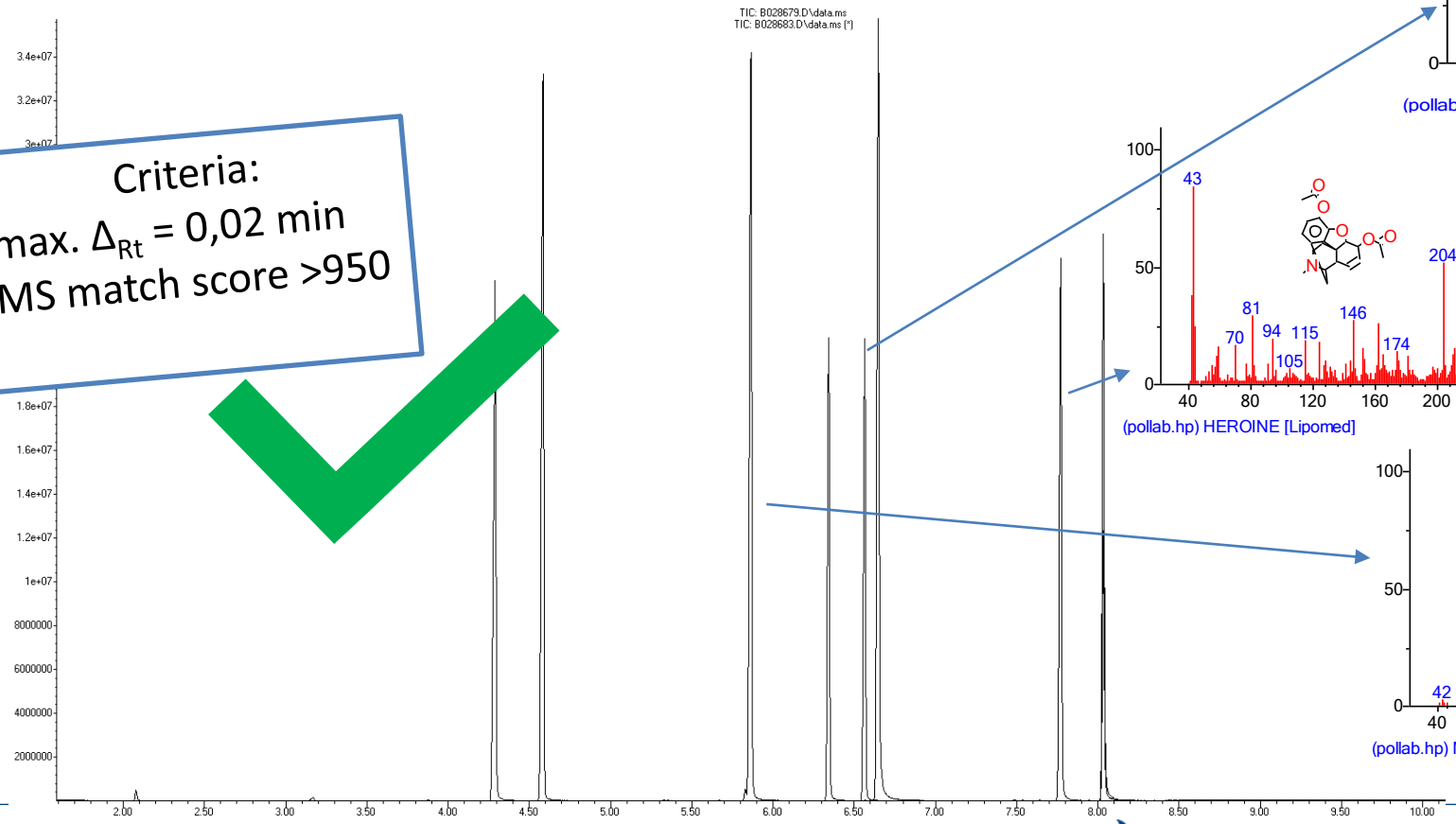
1939

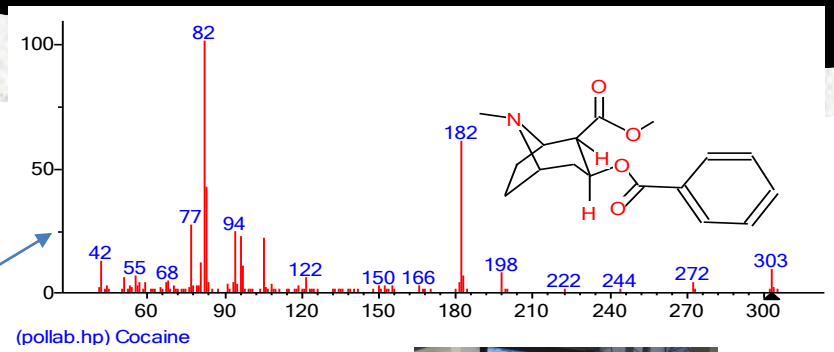
1980

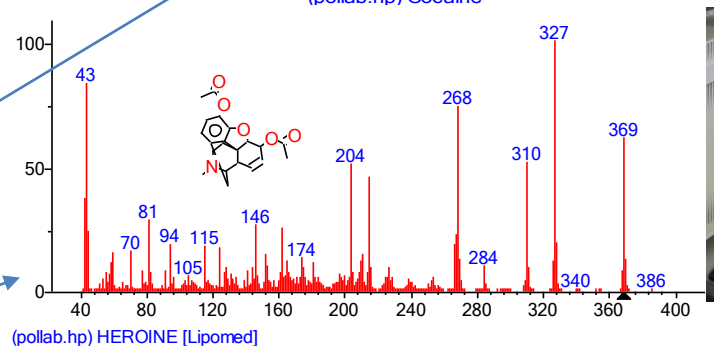
2023

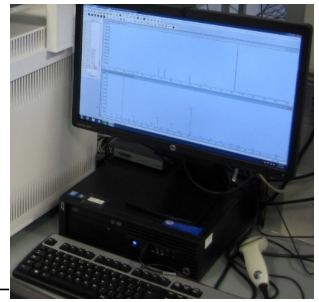
Drug analysis

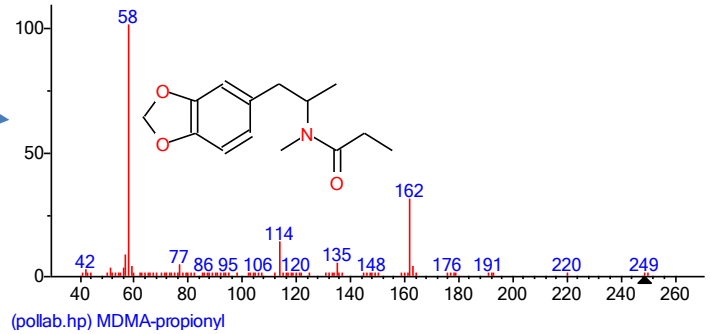
Criteria:
max. Δ_{Rt} = 0,02 min
MS match score >950





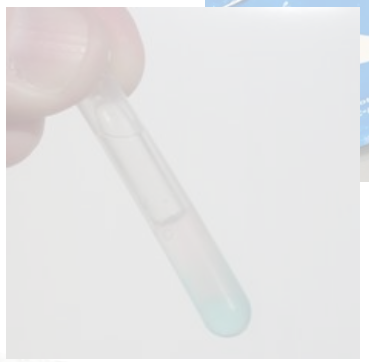


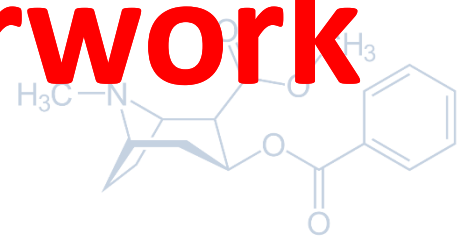


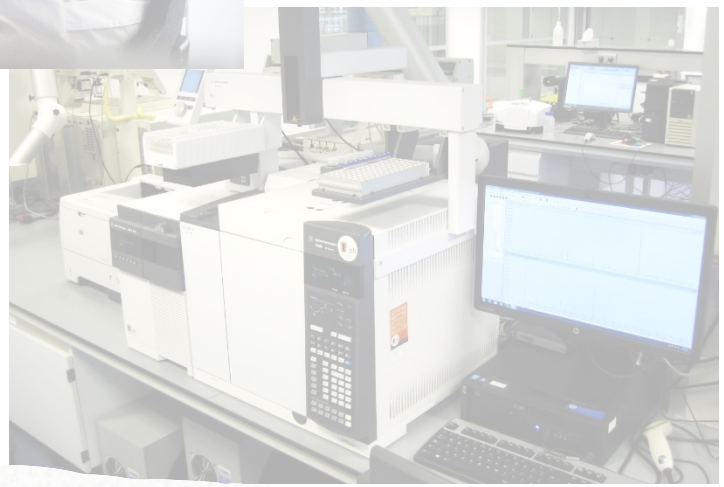


On-scene

Laboratory



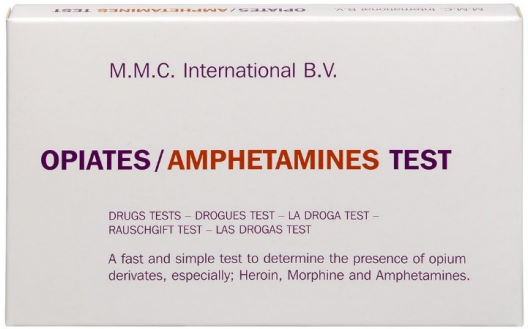




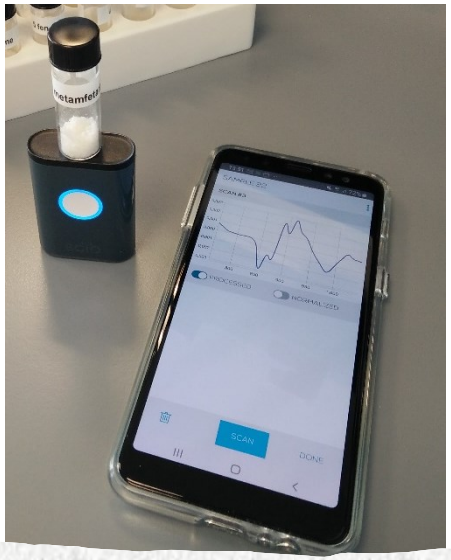
- transport
- paperwork
- time

The increasing amounts of drugs

1920 - 2015



> 2015



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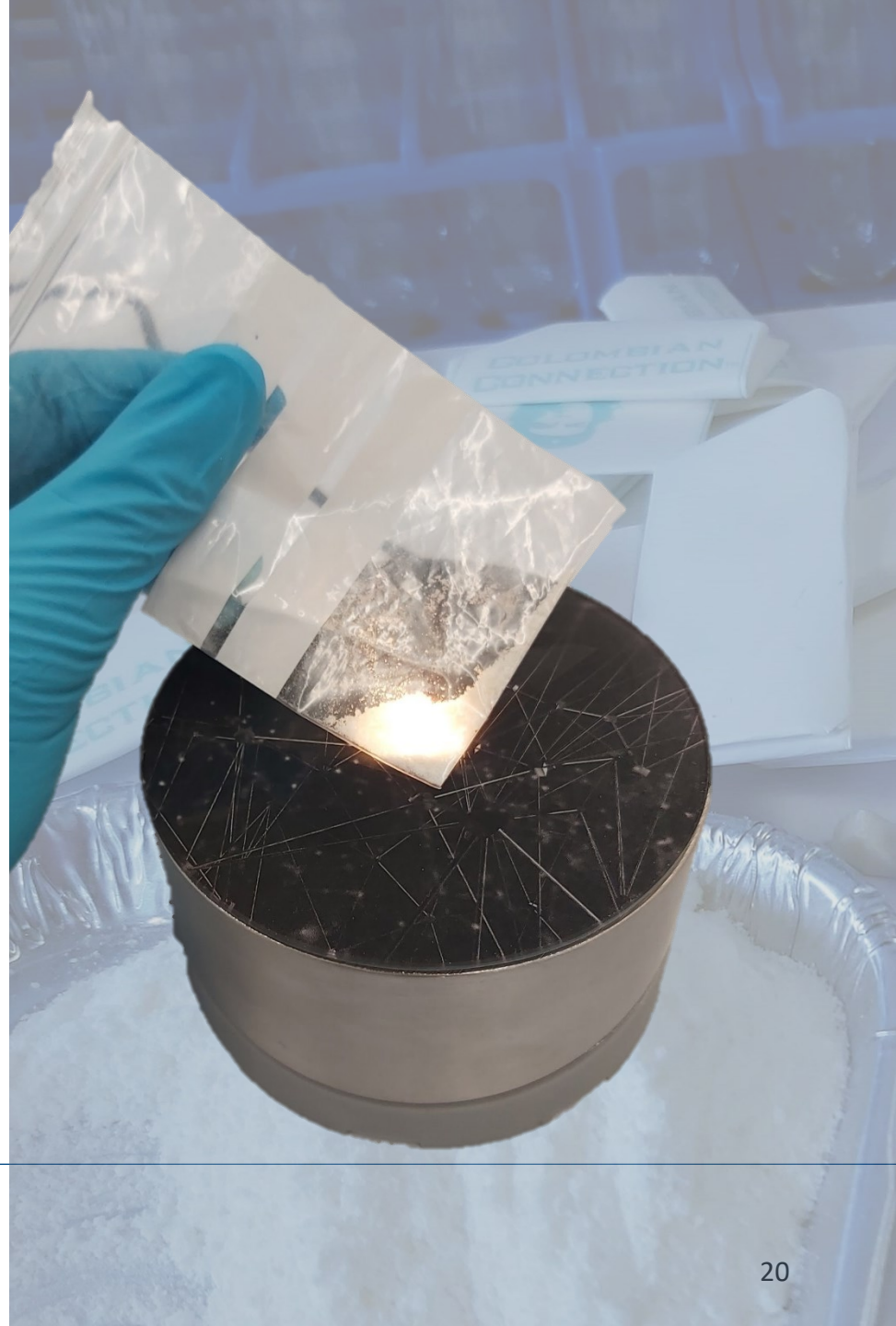
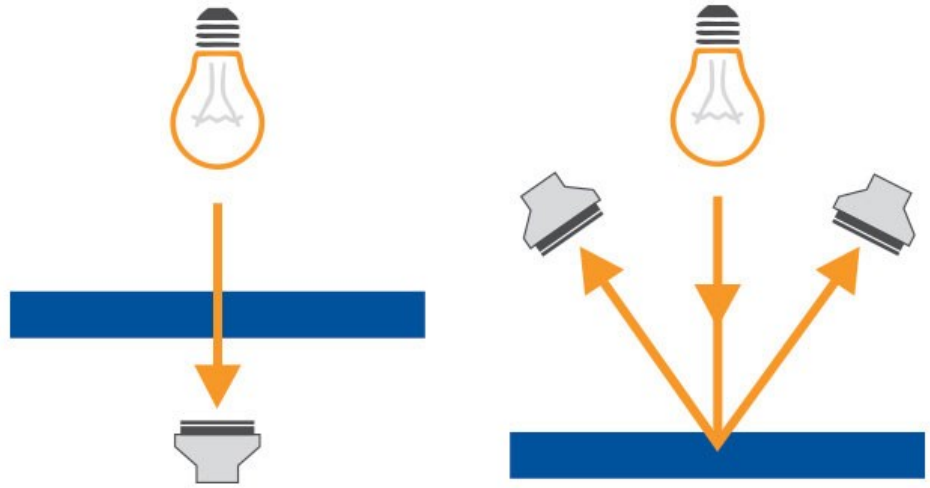


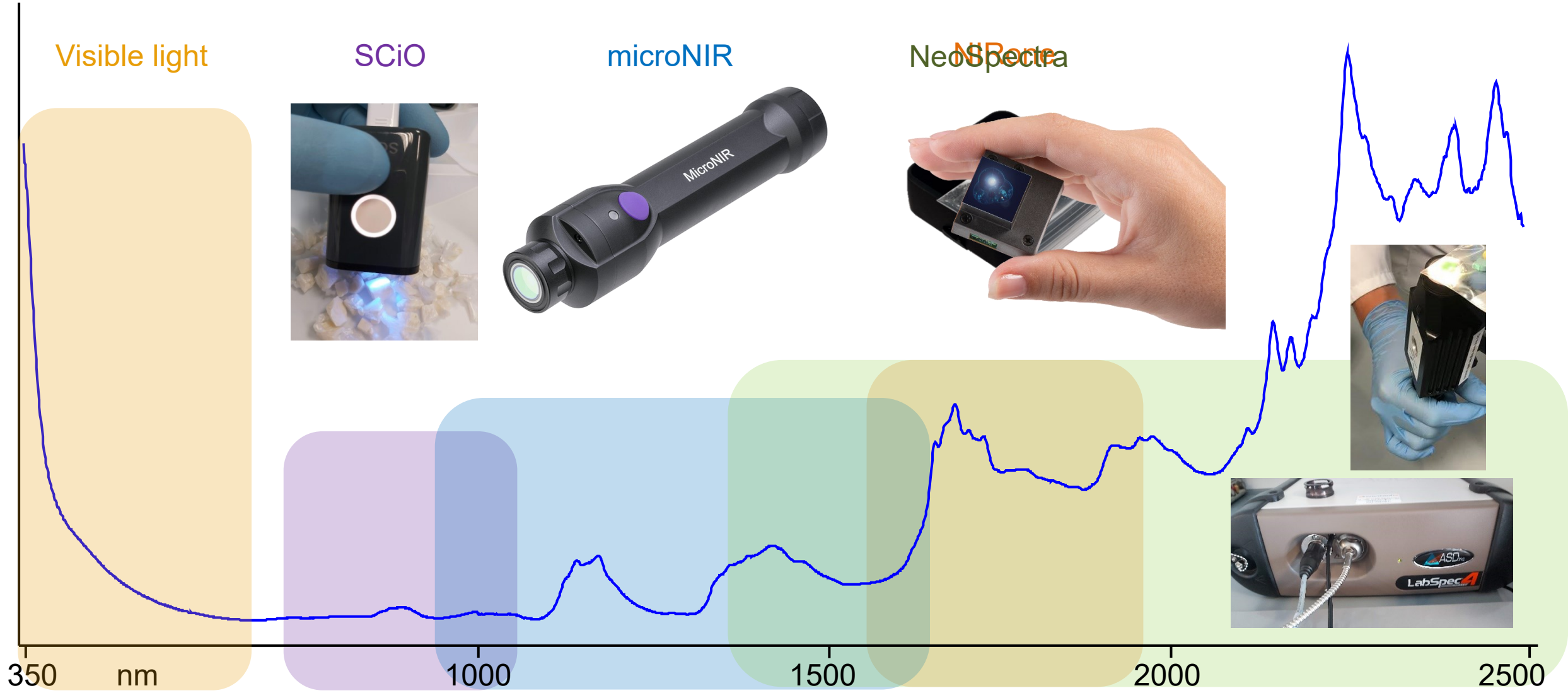
Near Infrared Spectroscopy

- ~700 – 2500 nm
- diffuse reflection *or* remission spectroscopy



absorbance reflection

source: FOSS analytics



SCiO
740 – 1070 nm

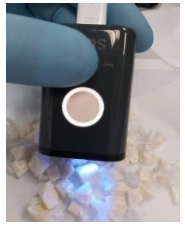
microNIR
950 – 1650 nm

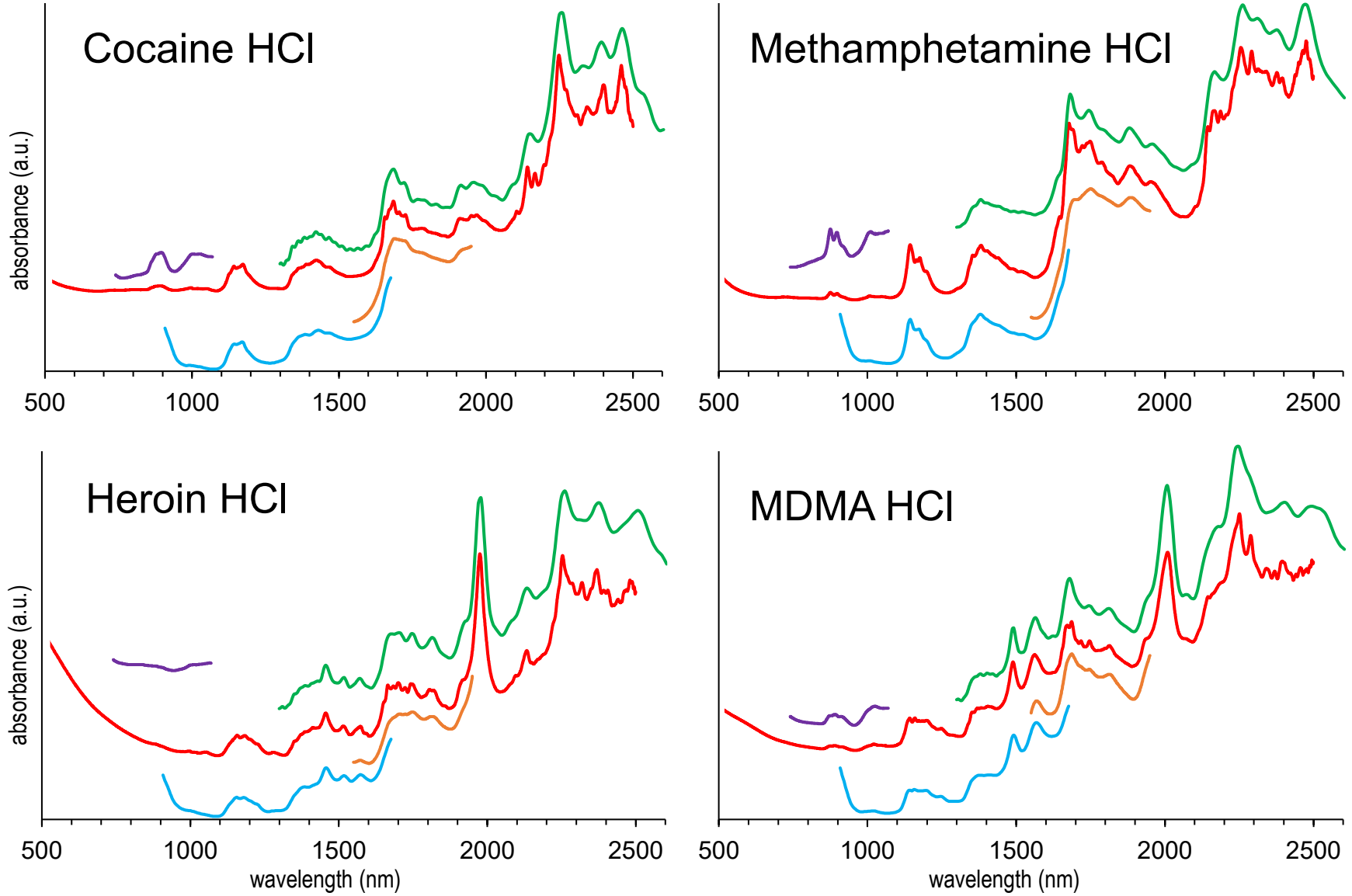
NeoSpectra
1300 – 2600 nm

ASD LabSpec4
350 – 2500 nm

Cocaine HCl

MicroNIR



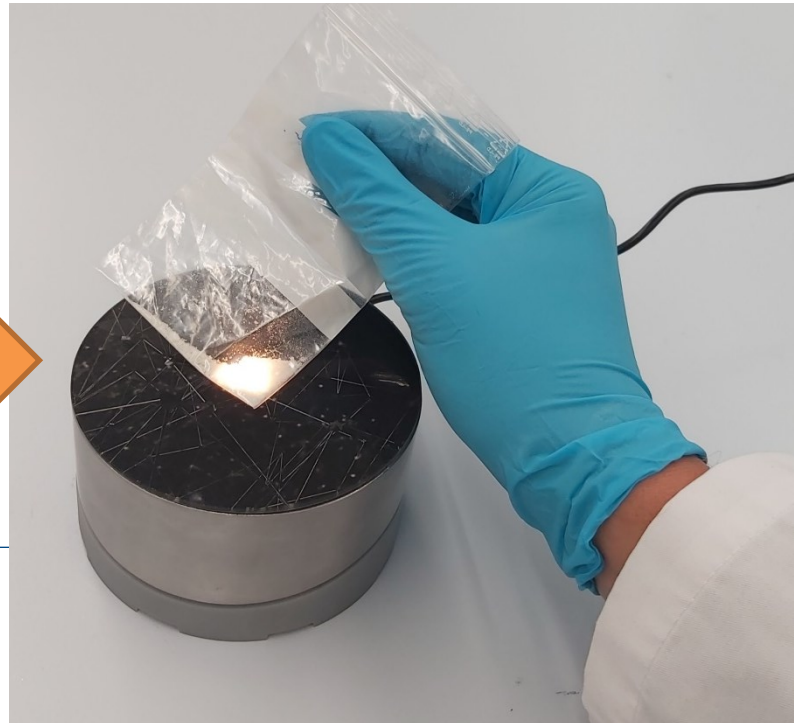

Cocaine HCl
Methamphetamine HCl
Heroin HCl
MDMA HCl
absorbance (a.u.)
absorbance (a.u.)
500
1000
1500
2000
2500
wavelength (nm)
wavelength (nm)

PowderPuck Illicit drug sensor

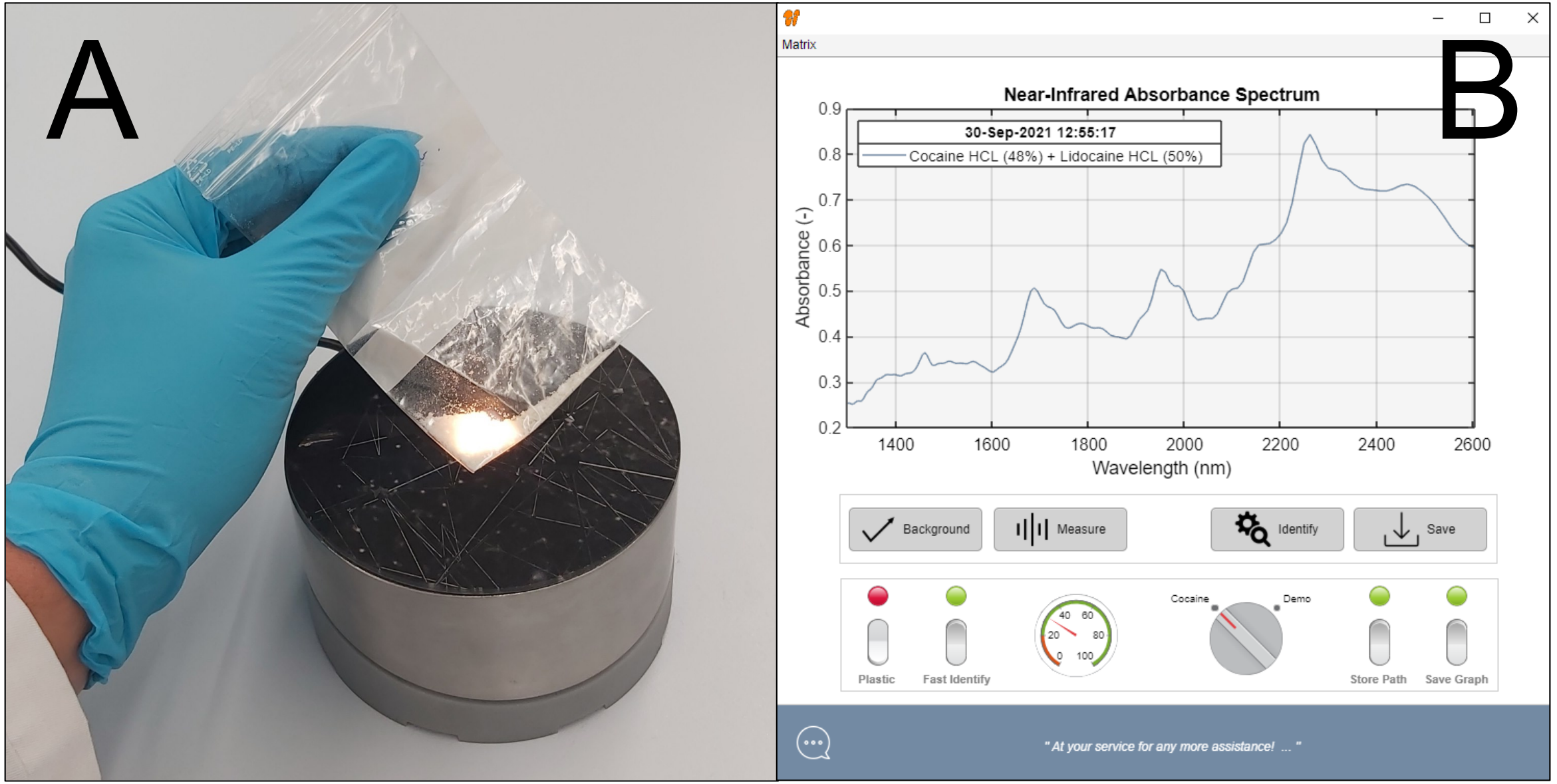
- NeoSpectra NIR sensor
  - 1300 – 2600 nm
  - Detector: miniaturized (MEMS) Michelson interferometer

Henk-Jan Ramaker
data scientist

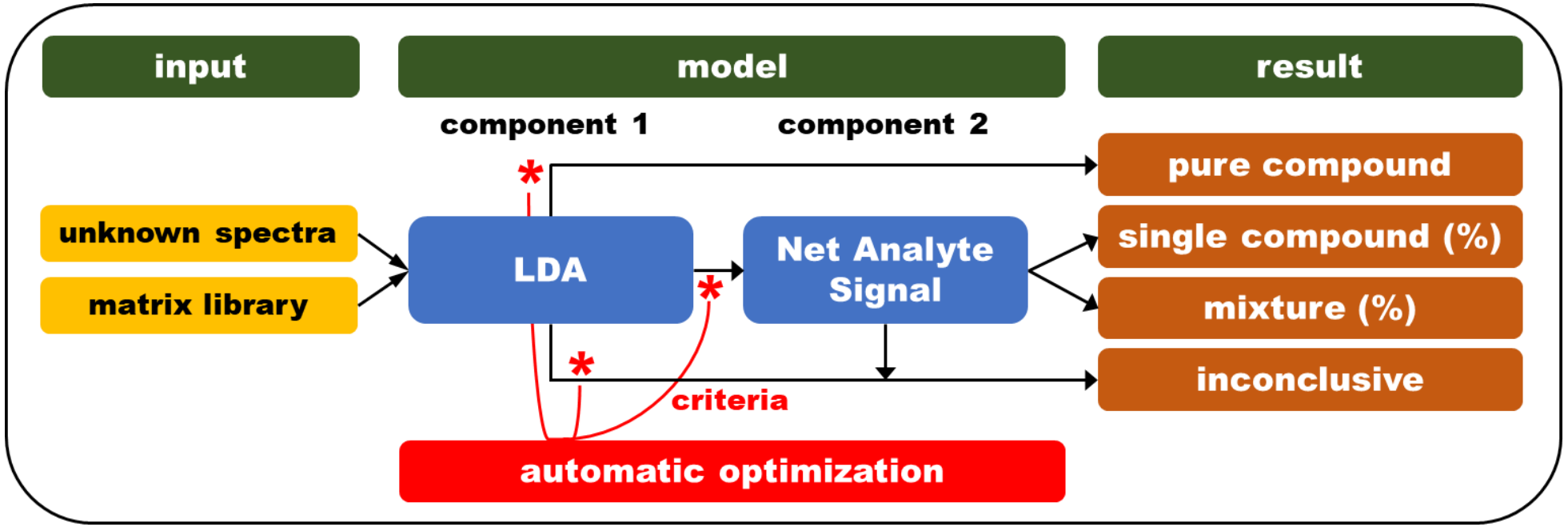
- Data model optimized for forensic setting
  - Focus on medium complexity mixtures
  - Calibration-light approach: only reference spectra needed
  - Multi-stage classification model



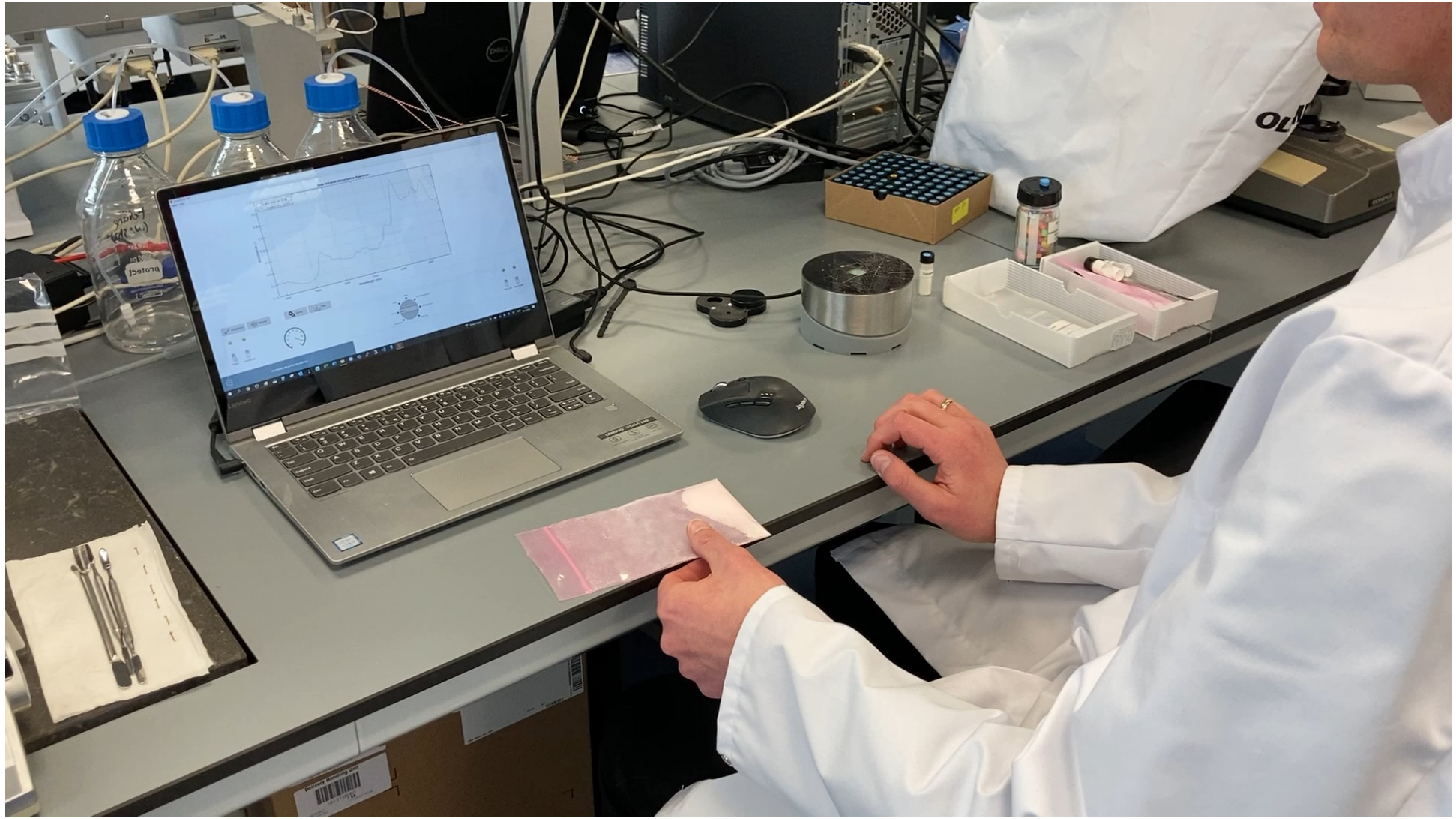
TIPb

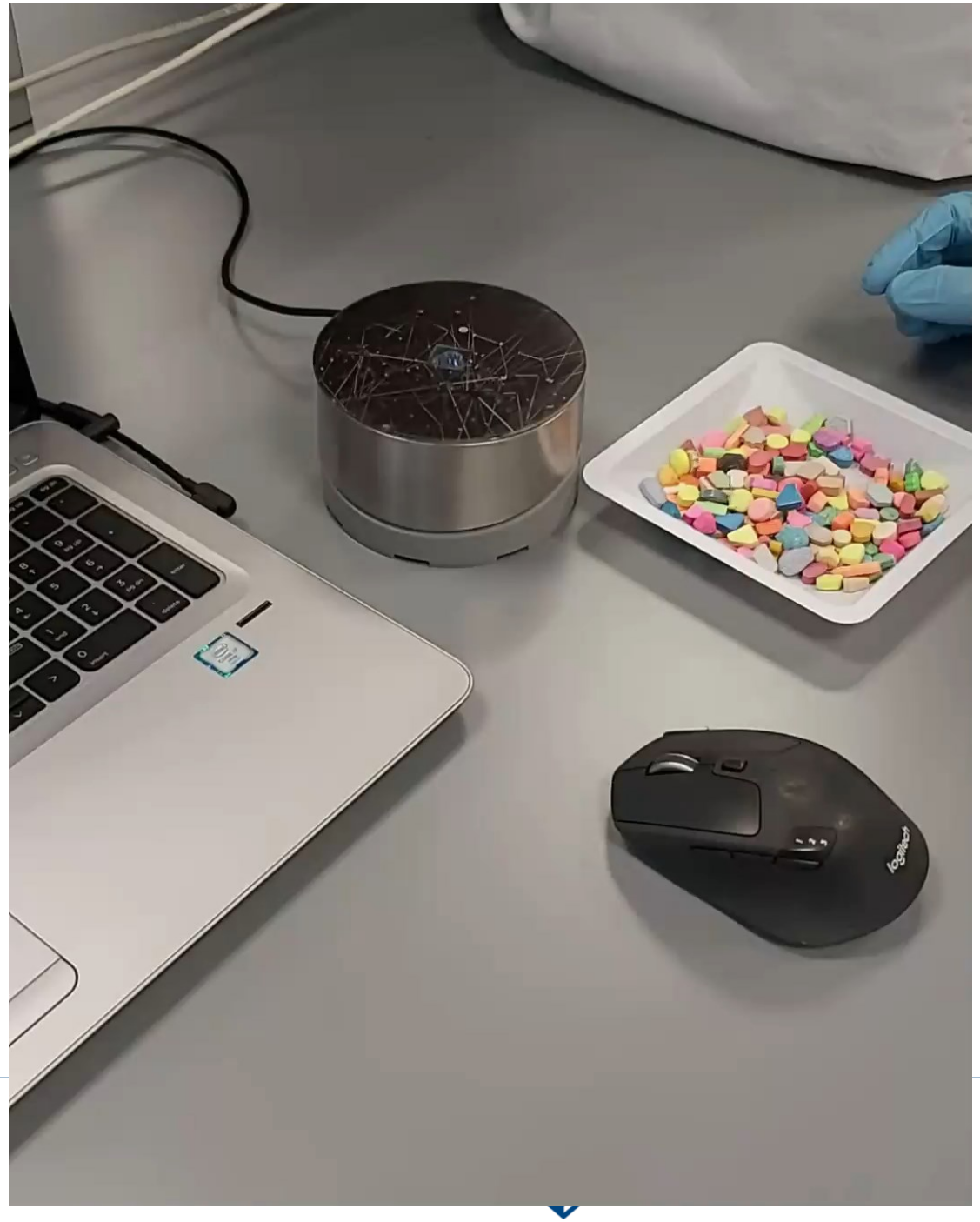

A
B
Matrix
Near-Infrared Absorbance Spectrum
30-Sep-2021 12:55:17
Cocaine HCL (48%) + Lidocaine HCL (50%)
Absorbance (-)
Wavelength (nm)
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
1400
1600
1800
2000
2200
2400
2600
Background
Measure
Identify
Save
Plastic
Fast Identify
40
60
20
80
0
100
Cocaine
Demo
Store Path
Save Graph
" At your service for any more assistance! ... "

Identification model



PowderPuck portable NIR spectrometer





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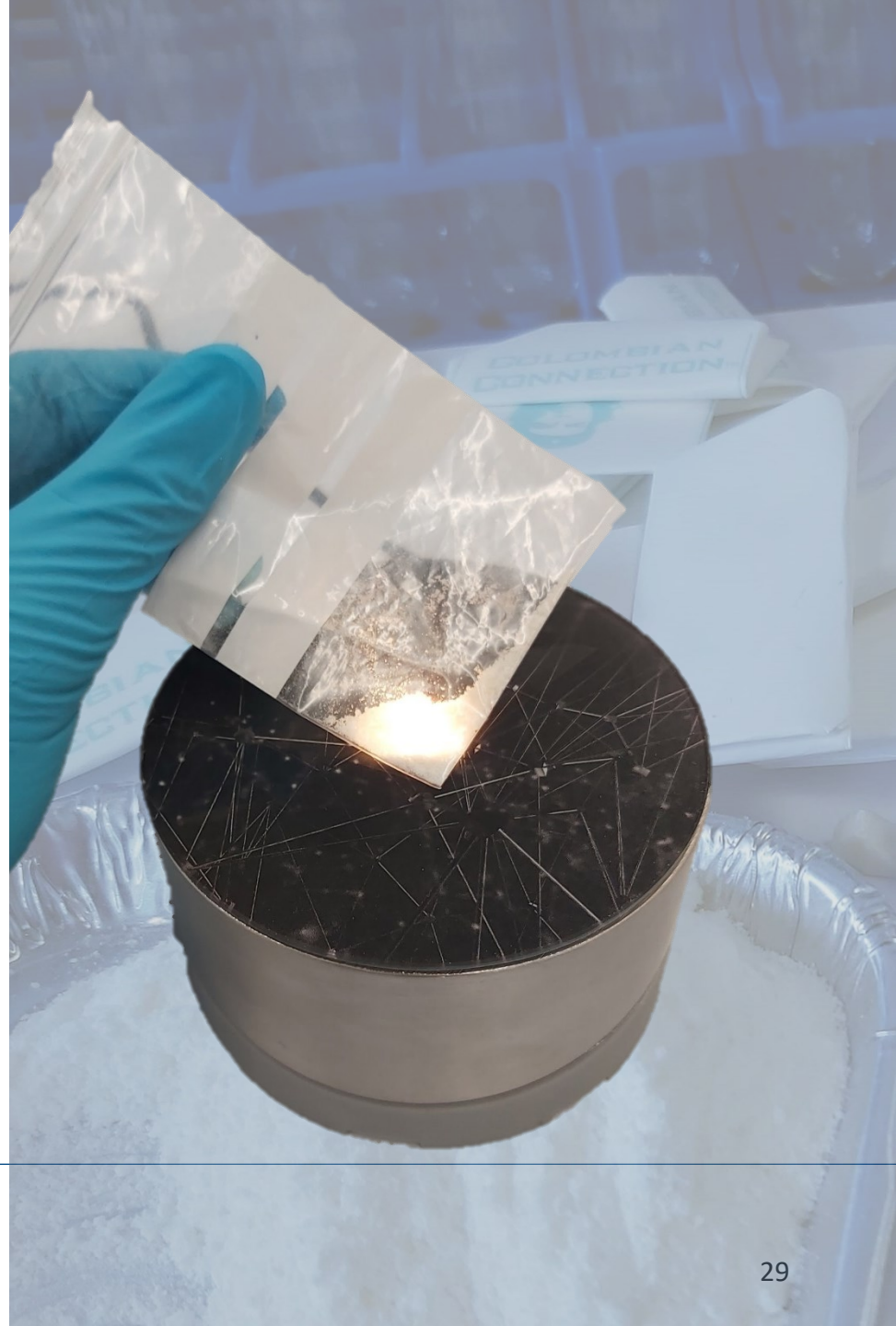


False positives & False negatives

520 different forensic samples

281 different ‘other’ samples
- designer drugs
- pharmaceuticals
- household chemicals

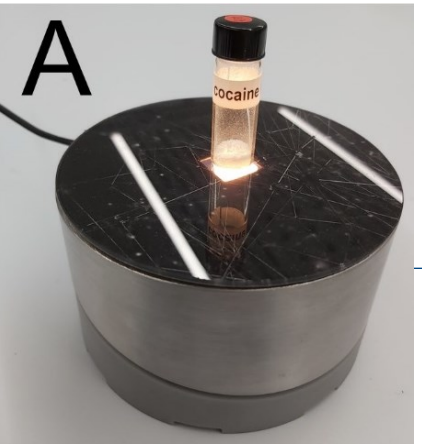
identity	PowderPuck result							
	cocaine	MDMA	ketamine	methamp	amph	heroin	other	inconclusive
cocaine	**98% (574)**	0% (0)	0% (1)	0% (0)	0% (0)	0% (0)	1% (4)	2% (9)
MDMA	0% (0)	**100% (48)**	0% (0)	0% (0)	0% (0)	0% (0)	0% (0)	0% (0)
ketamine	0% (0)	0% (0)	**94% (48)**	0% (0)	0% (0)	0% (0)	0% (0)	6% (3)
methamphetamine	0% (0)	0% (0)	0% (0)	**100% (15)**	0% (0)	0% (0)	0% (0)	0% (0)
amphetamine	14% (7)	0% (0)	0% (0)	0% (0)	**61% (31)**	0% (0)	0% (0)	25% (13)
heroin	0% (0)	0% (0)	0% (0)	0% (0)	0% (0)	**89% (8)**	0% (0)	11% (1)
other	0% (1)	0% (0)	0% (0)	0% (0)	0% (2)	0% (0)	**16% (136)**	**84% (704)**

False Negatives

- Low level drug samples (~5 wt%)
- Incomplete matrix libraries (amphetamine)
- Physical properties (chunks)

False Positives

- Physical properties (chunks) in combination with diluted samples
- Multiple adulterated samples

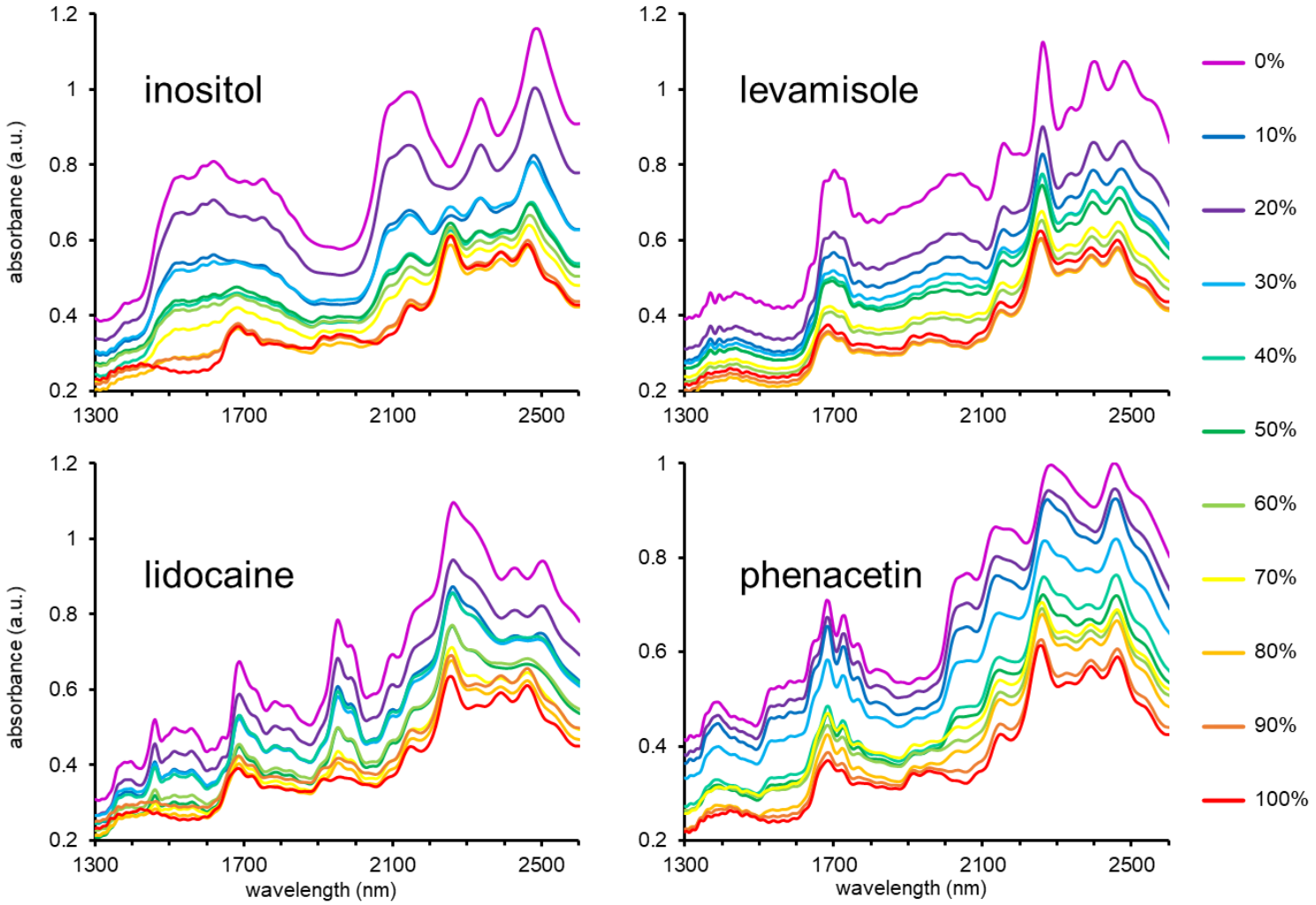


False positives & False negatives

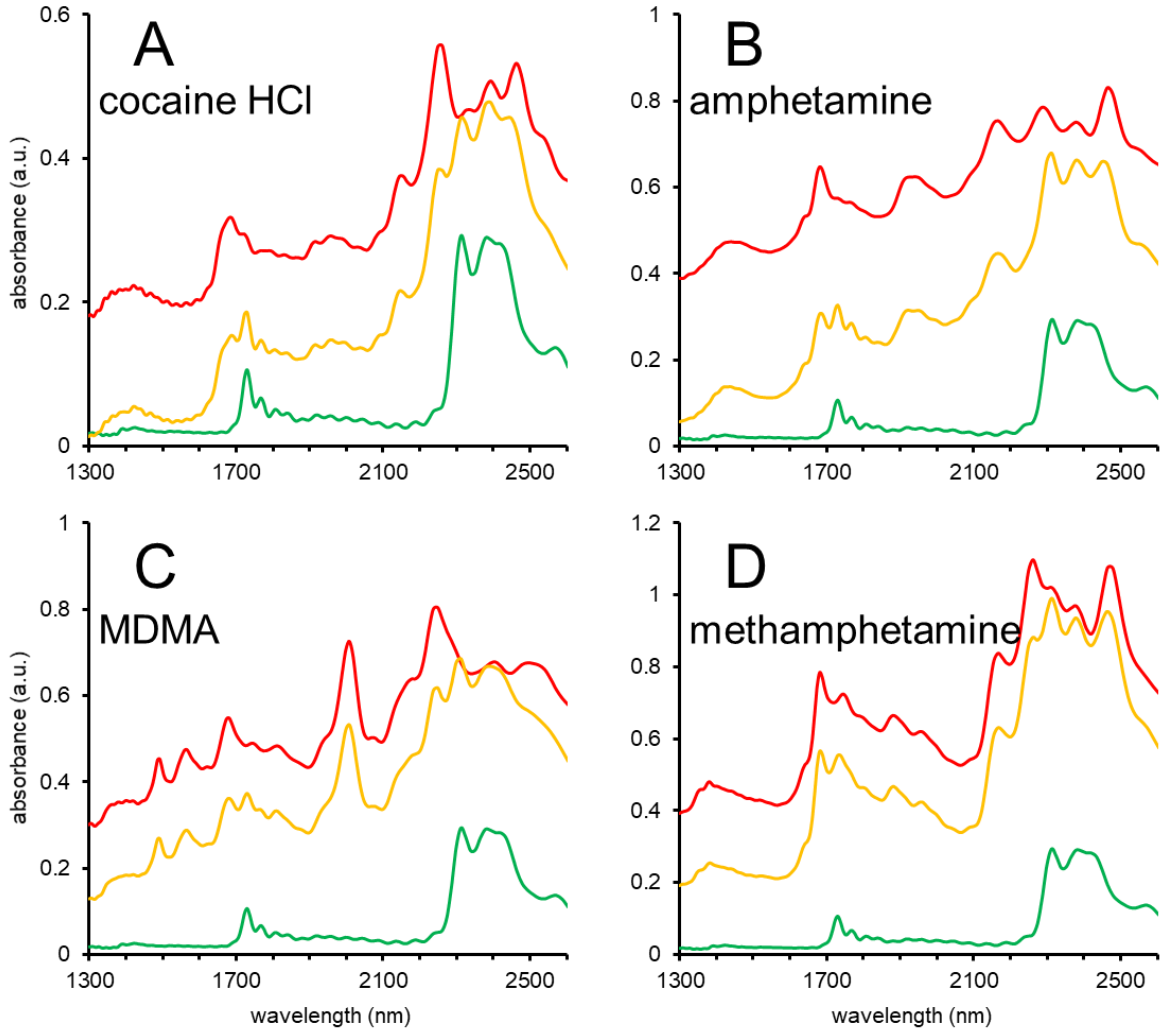
- Binary cocaine mixtures
- 0 – 100 wt%

only 10 wt% (4 out of 24 scans)

set K	cocaine	other
cocaine	236	4
other	0	24



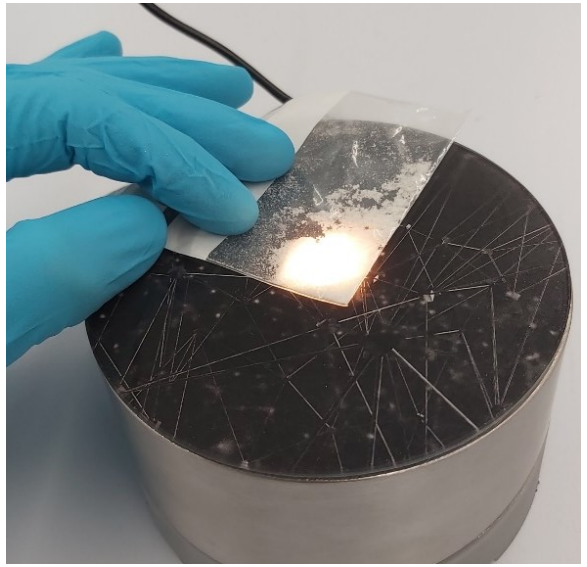
Influence of LDPE plastic

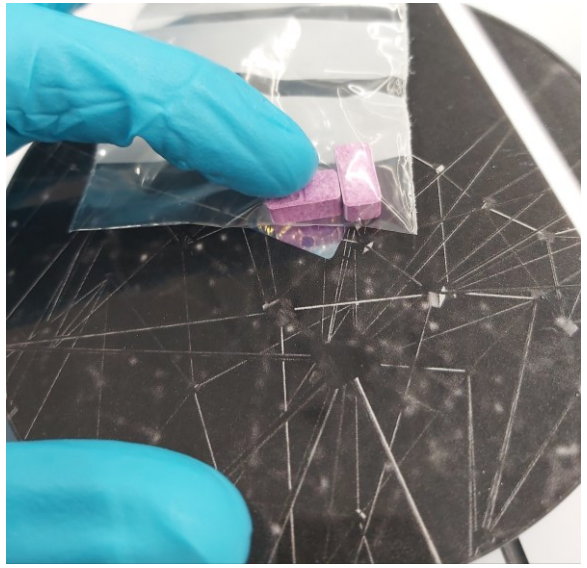


Pure drug

Drug in plastic bag

LDPE plastic





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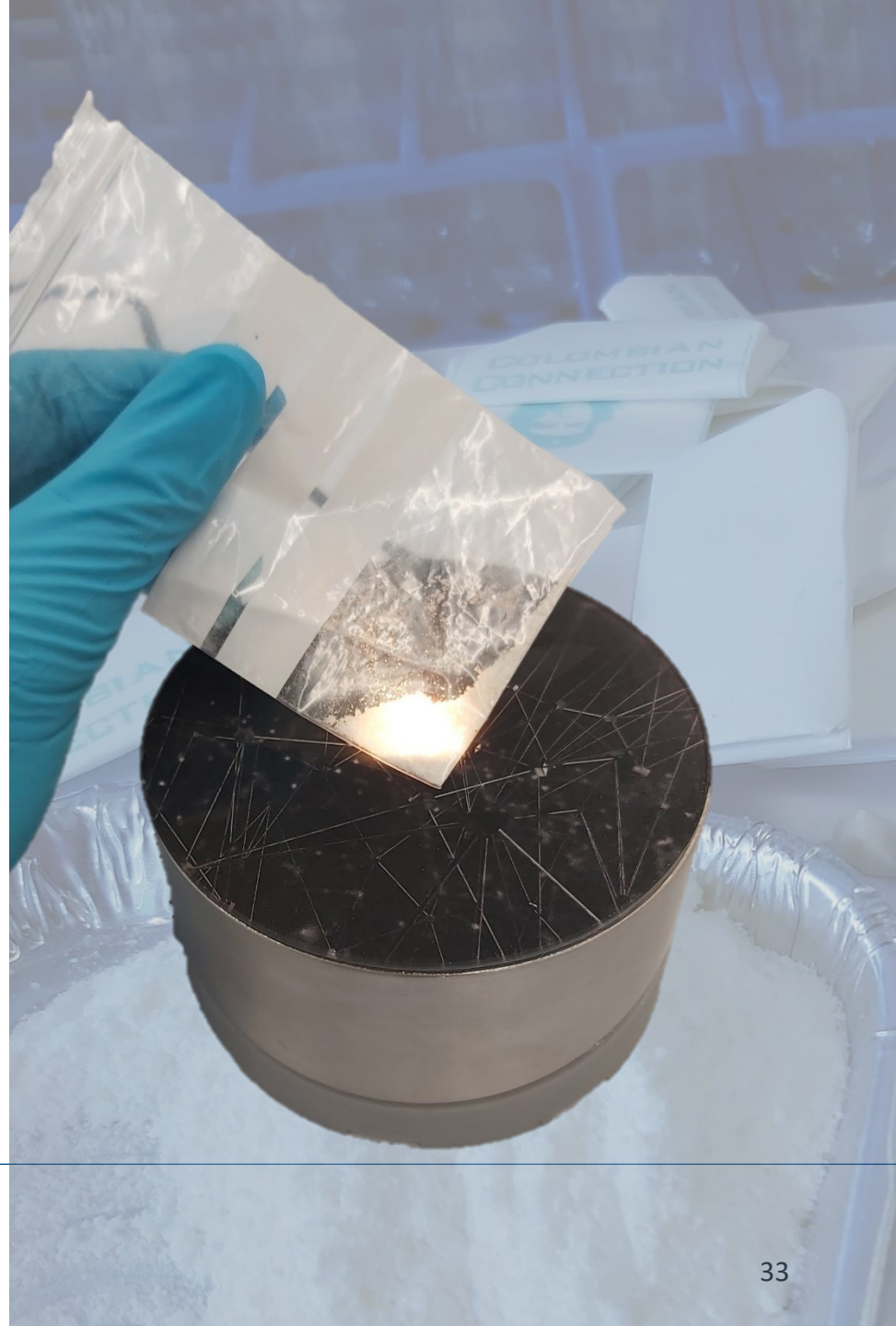

Conclusions

- Rapid 5 second drug detection by portable NIR is possible
- Wise sensor selection and model design improves quality
- 99.6% TN (0.4% FP) and 97.6% TP rate for cocaine
- Similar figures when analyzed through plastic

ALSO:

- 0% FP possible using a threshold of 23 wt% drugs

Flawless (court-admissible) drug detection?

1737 unique samples tested

cocaine, heroin, MDMA, non-drugs
powders, tablets, through packaging

- 0% FP possible
  - using a threshold of 23 wt% drugs
- ~1% FN possible
  - using expert knowledge on appearance
  - using a 2-stage approach: inconclusive -> sent to lab

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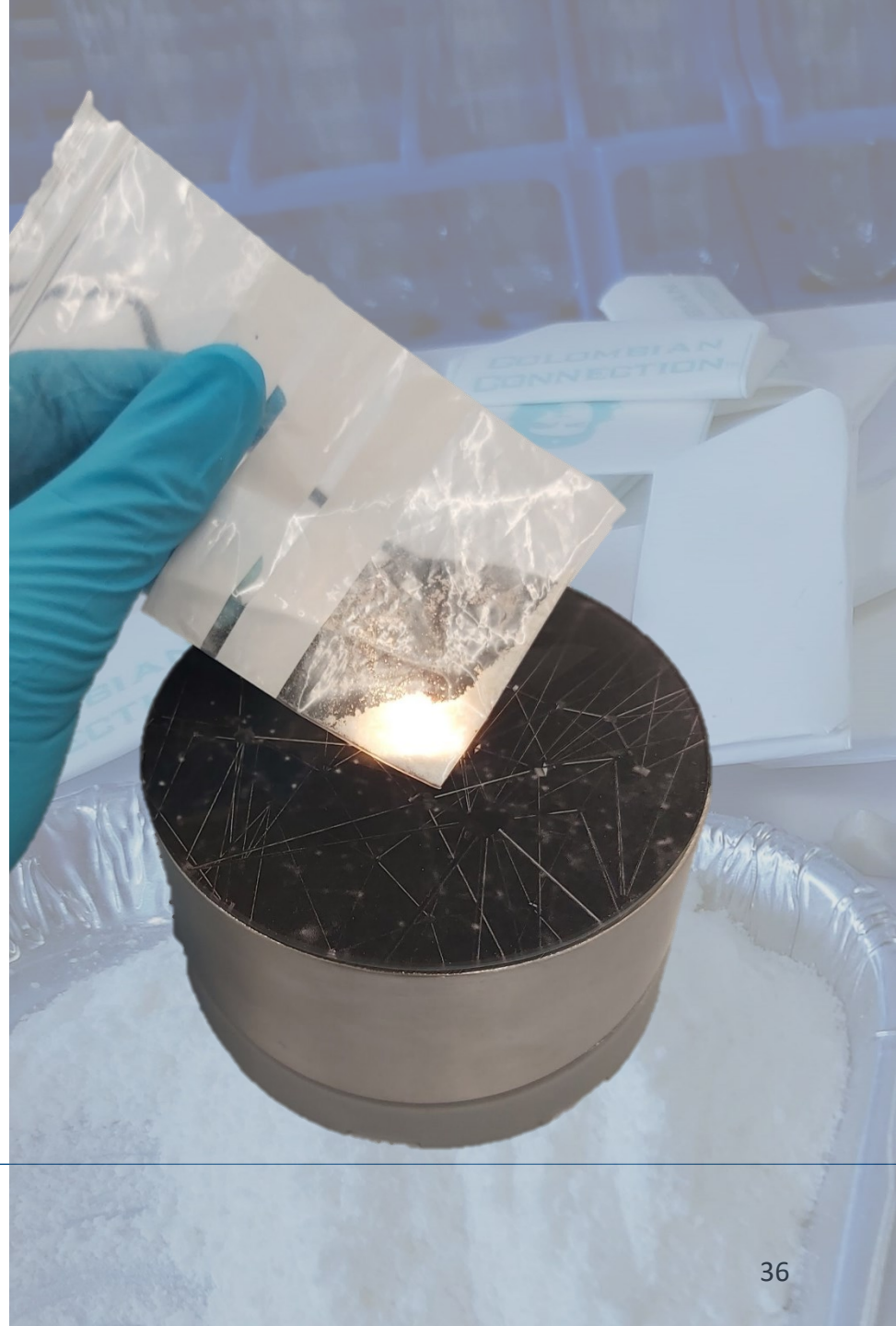
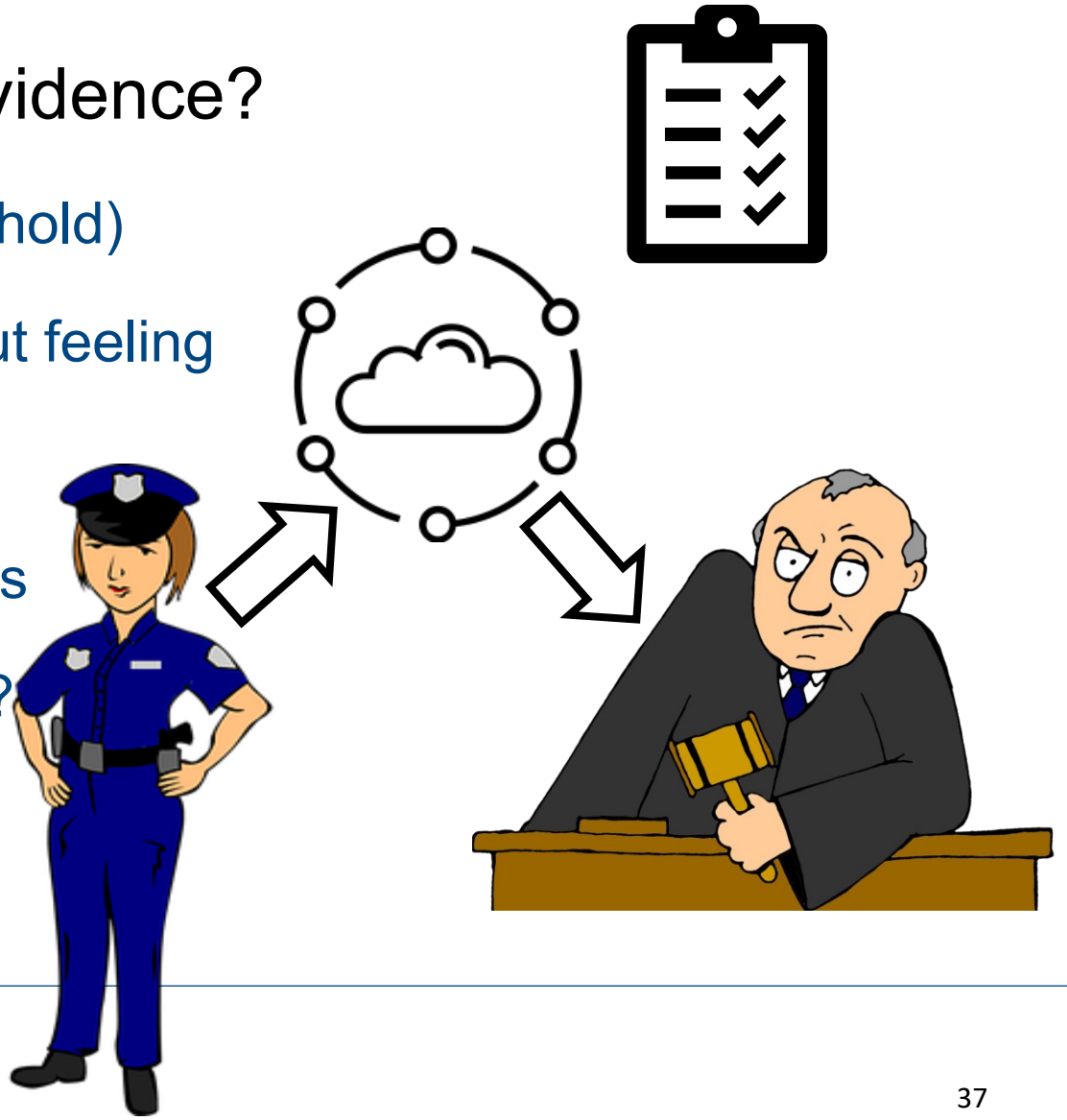
- Conclusions
- **Future Outlook: towards implementation**



Future outlook

- Sufficient evidential value for court evidence?
  - No FP? (1000+ samples, at 23wt% threshold)
  - Not chromatography-based… expert's gut feeling
  - Executed by non-laboratory trained staff
  - Not compliant with SWGDRUG guidelines
  - Two portable techniques? NIR + Raman?
- Efficient sensor platform



Towards an analytical platform

A platform facilitates the identification of illicit drugs

Just like a train platform facilitates travelling

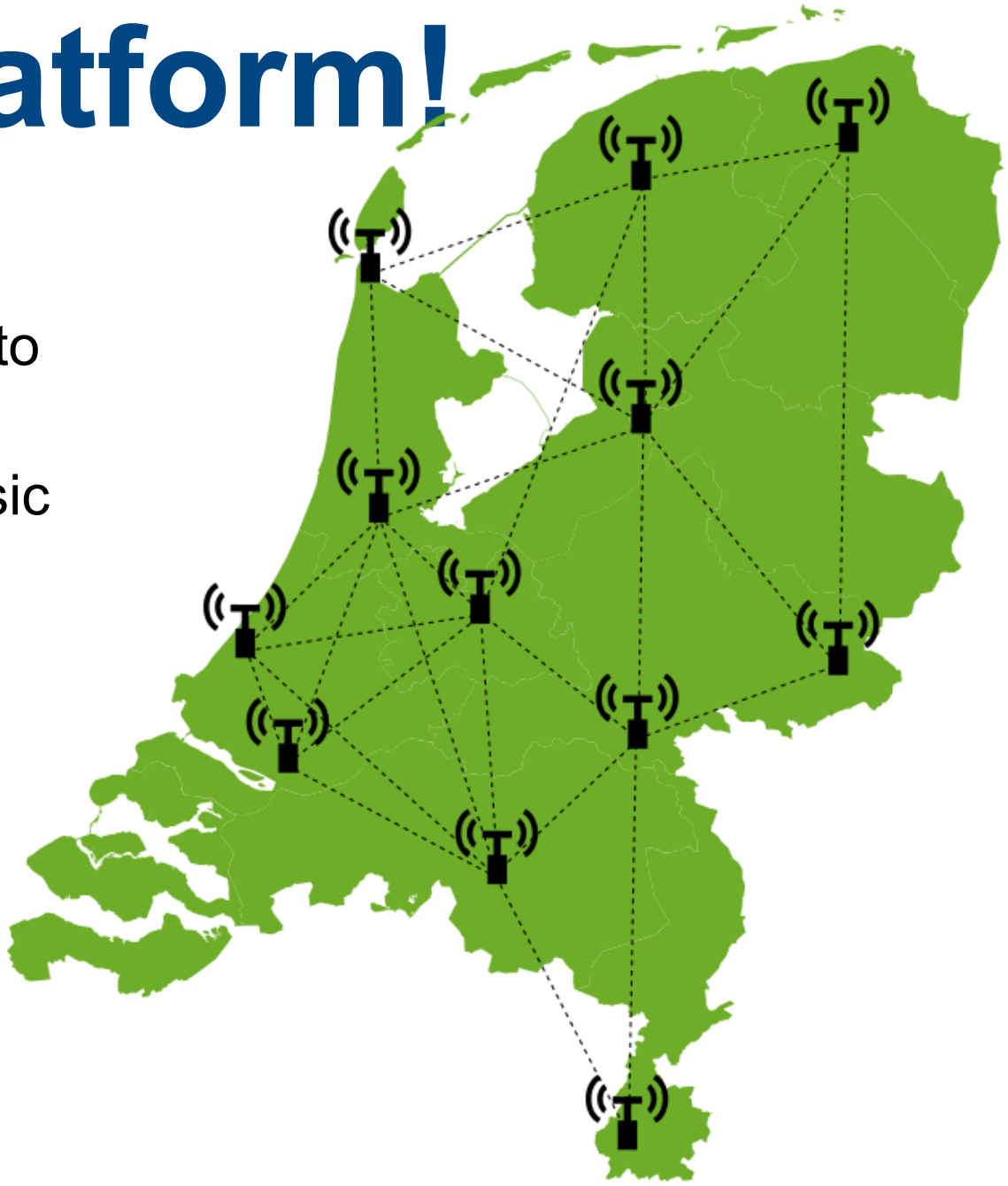
- ✓End-Users
- ✓Platform manager
- ✓Power-Users
- ✓Certification
- ✓Data Modelling
- ✓Research & Development
- ✓Entrepreneurship
- ✓System Integration
- ✓Sample storage
- ✓Analytical chemistry
- ✓Software
- ✓Sensor technology

Analytical Platform for Illicit Drugs Identification

Analytical Platform for Illicit Drugs Identification

Leverage this platform!

- The ANALYTICAL platform can be used to create a sensor network
- This network can help to globalize forensic investigation expertise



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