

# Using FT-IR for Drug Checking in the Netherlands

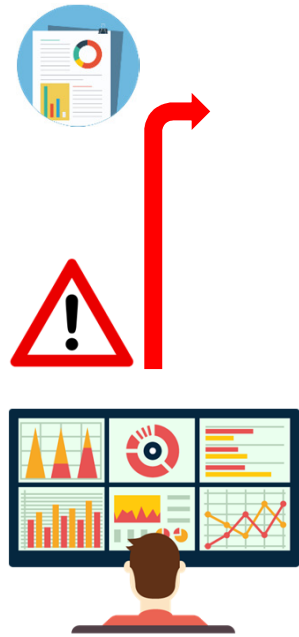
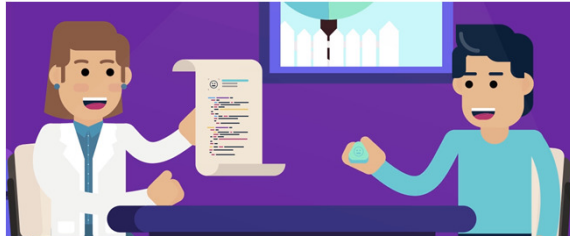
**A reflection of two years working experience.**

Ruben Vrolijk, Drug Information & Monitoring System



# Quick introduction to DIMS

Drug information and monitoring system



DIMS

FT-IR

Results

Perks & Limitations

Future plans

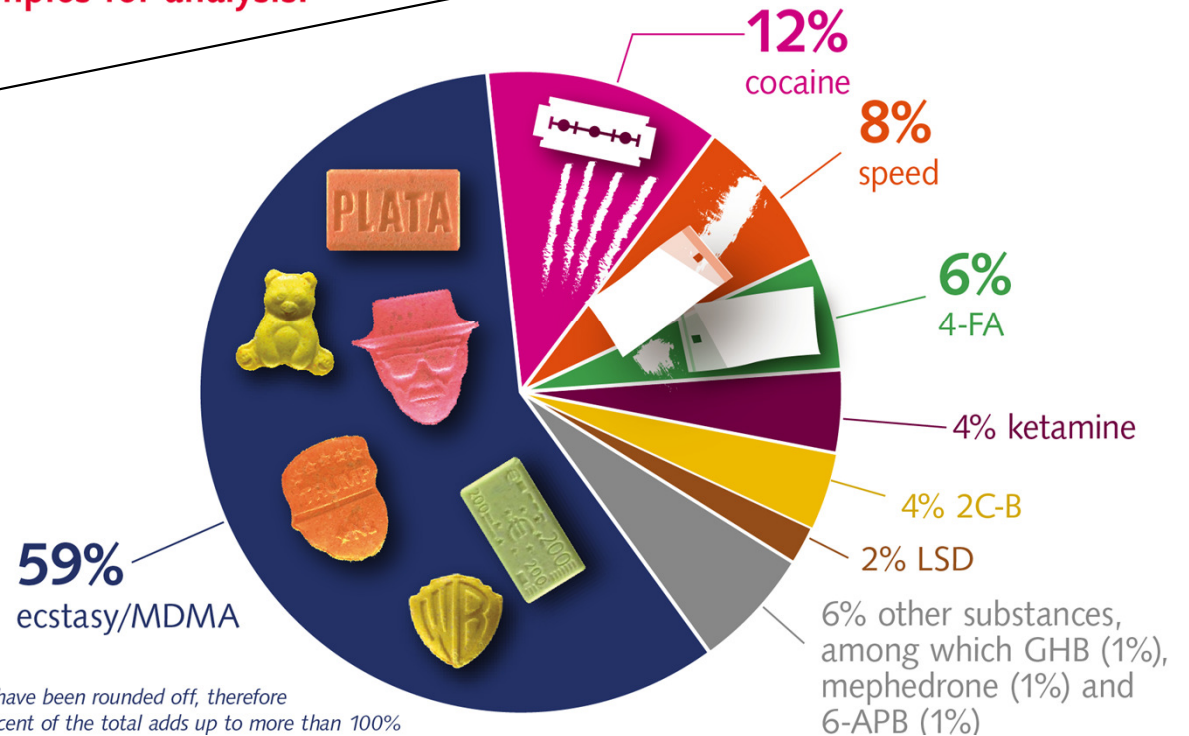
# Quick introduction to DIMS

How do we supply the monitor and DIMS-users with significant information when GC-MS/LC-DAD analysis is not possible?

125 samples/week: GC-MS/LC-DAD  
11,963/52 = 230 samples/week  
100 samples/week 'too much'



In 2017, 12,161 visitors handed in 11,963 samples for analysis.



DIMS

FT-IR

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# Quick introduction to DIMS

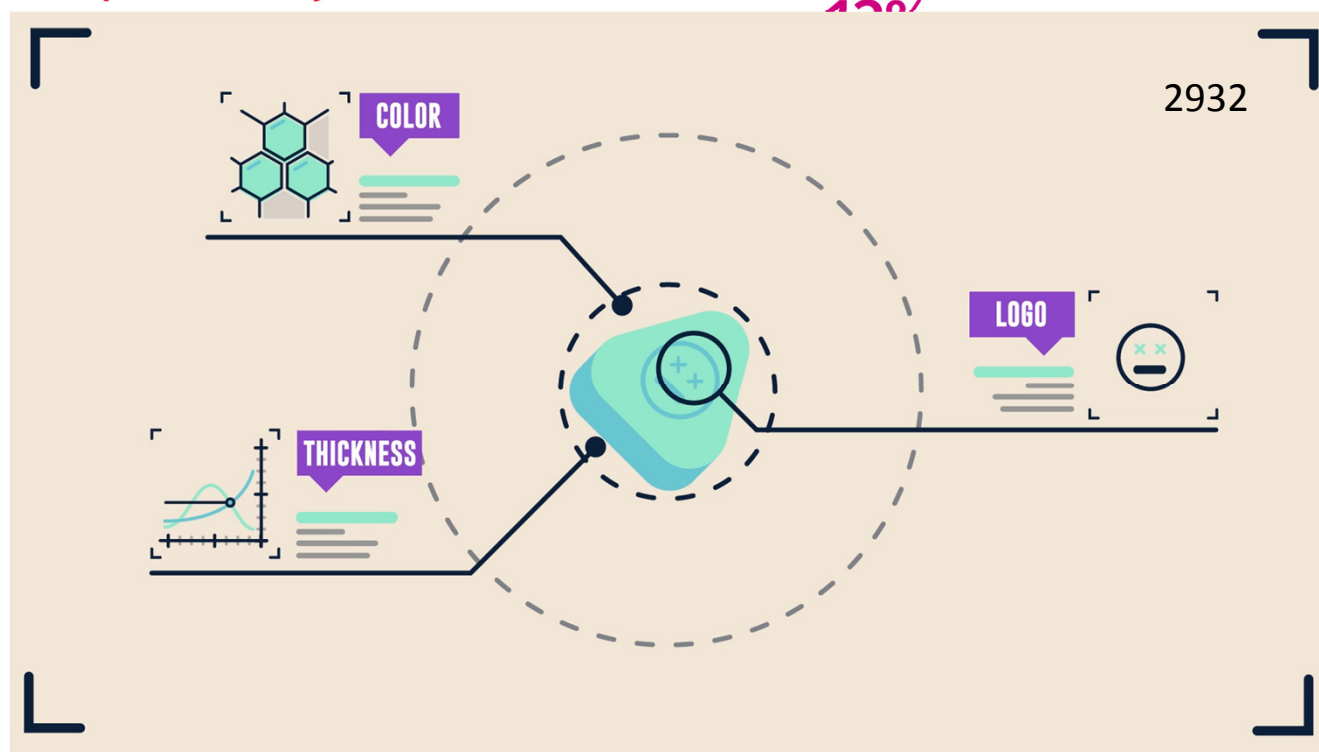
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DIMS

FT-IR

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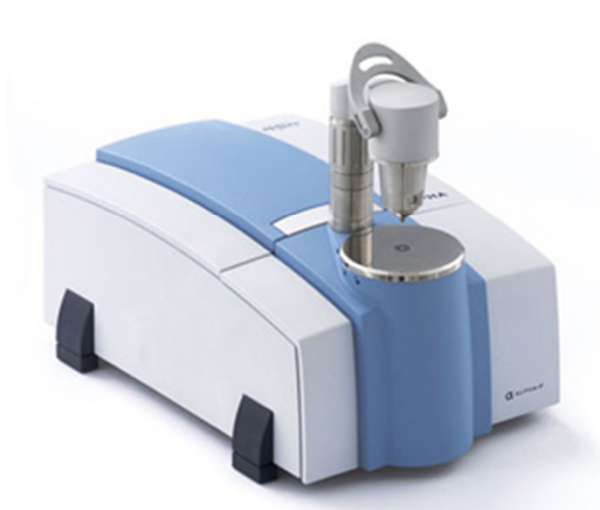


Results

Perks & Limitations

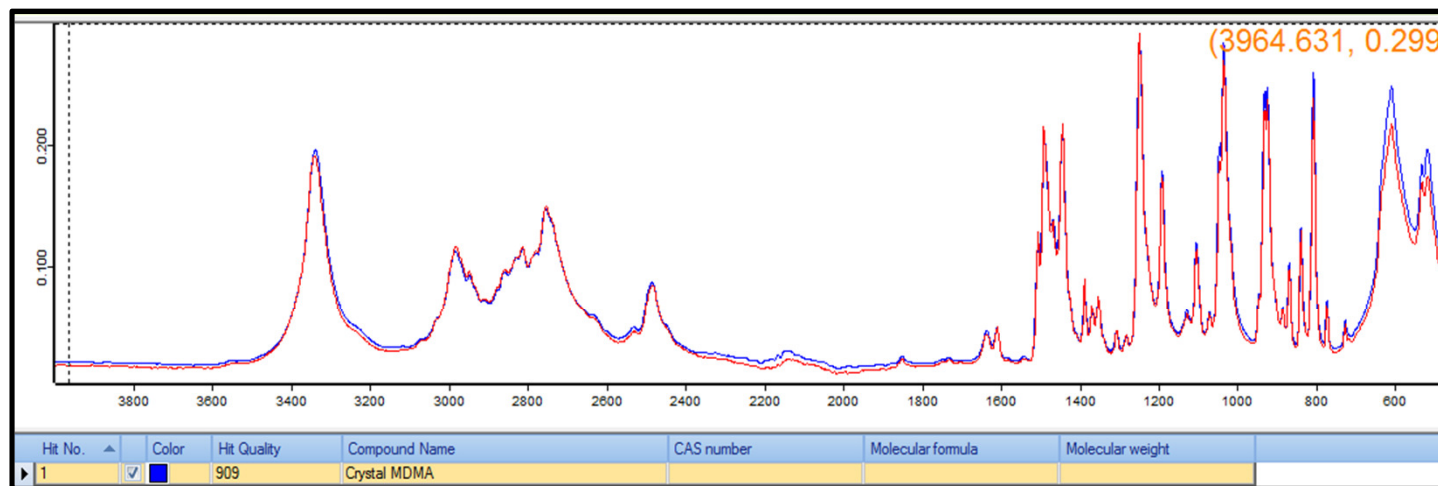
Future plans

# FT-IR: Fourier Transform Infrared Spectroscopy

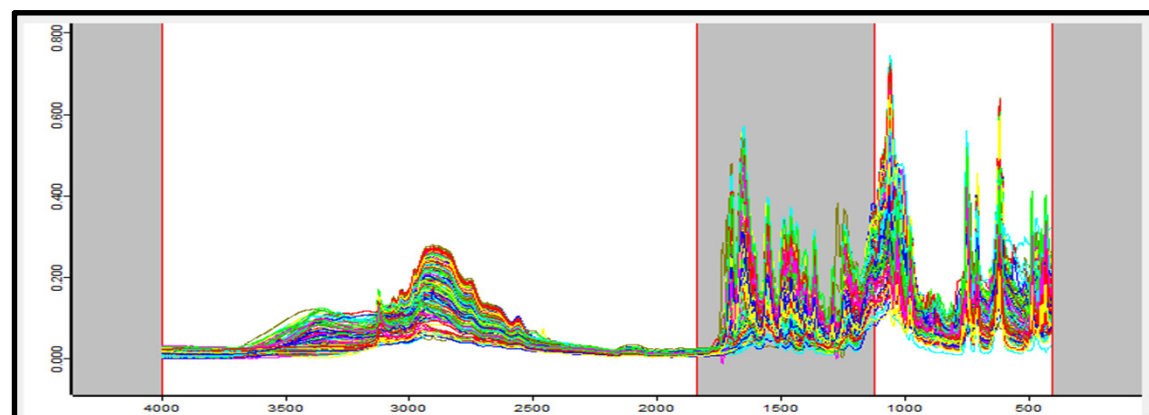


DIMS

FT-IR



Results



Perks & Limitations

Future plans

# FT-IR: Fourier Transform Infrared Spectroscopy

- **Two years of working experience**
- **Reflect on 2017**
- **What FT-IR results did we produce?**
- **Which substances did we determine reliably?**
- **Which substances did the FT-IR miss?**



DIMS

FT-IR

Results

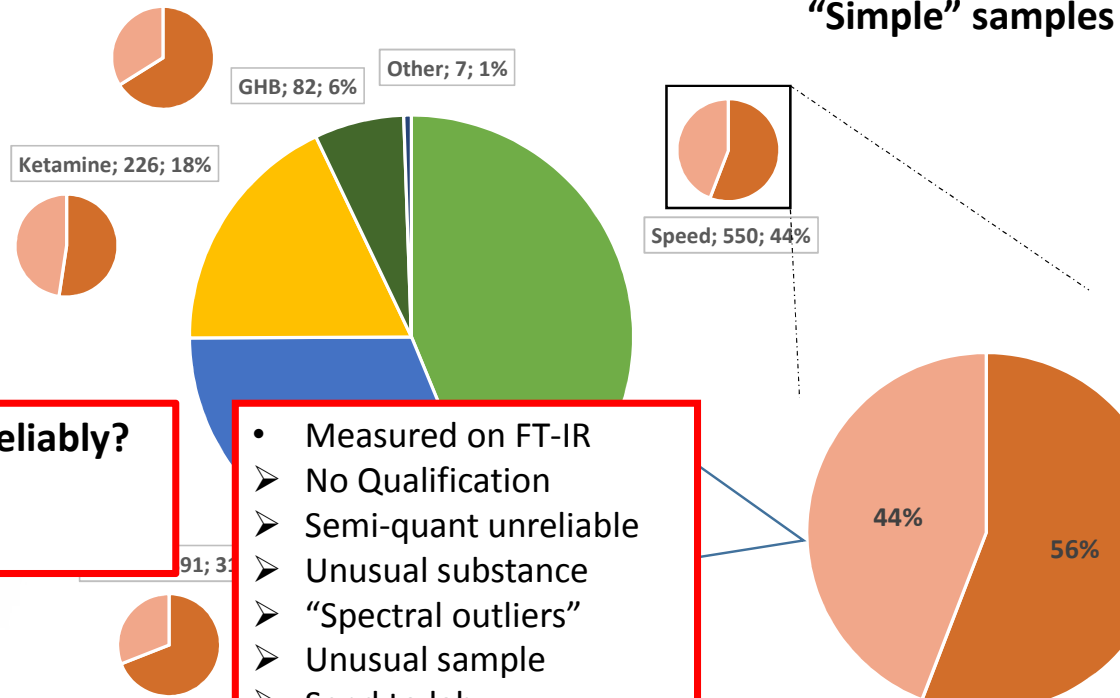
Perks & Limitations

Future plans

# FT-IR: Fourier Transform Infrared Spectroscopy

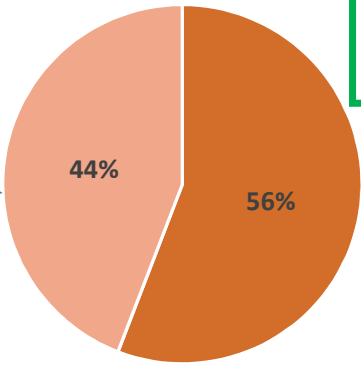
- Results of 2017
- 1256 samples
  - Only FT-IR

Samples determined by FT-IR in 2017



- Which substances did we determine reliably?
- Which substances did the FT-IR miss?

- Measured on FT-IR
  - No Qualification
  - Semi-quant unreliable
  - Unusual substance
  - “Spectral outliers”
  - Unusual sample
  - Send to lab



DIMS

FT-IR

Results

Perks & Limitations

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# Which substances did we determine reliably?

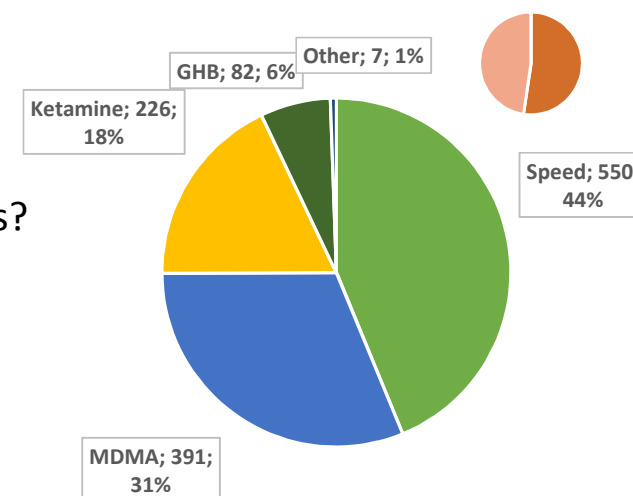
Cutoff values for single hit and mixture analysis.

- **Qualification of Amphetamine, MDMA, Ketamine and GHB very reliable (with correct settings)**
  - No false positives (because of cutoff values and quant. Models), n=398 in 2017
  - Mescaline
  - U-47700
  - 5-MeoDMT

But..... simple powders

How well does FT-IR do with mixtures and/or low concentrations?

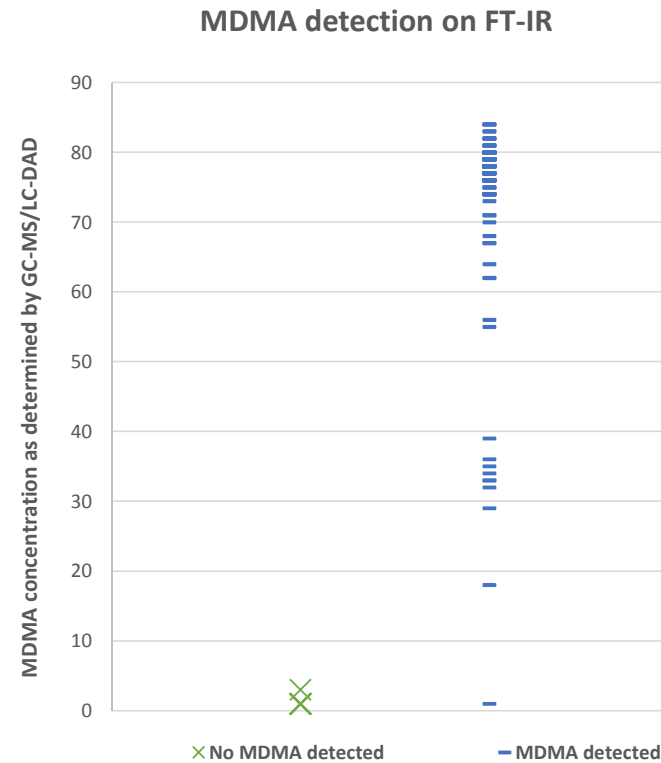
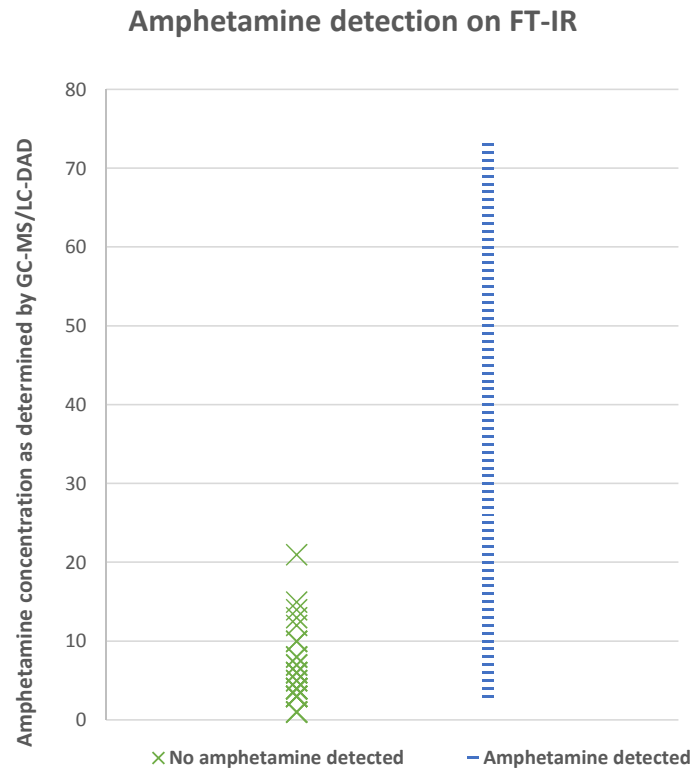
Lets look at false negatives.





# Which substances did the FT-IR miss? (optimal)

Every hit in single hit analysis or mix analysis counts as “detected”



DIMS

FT-IR

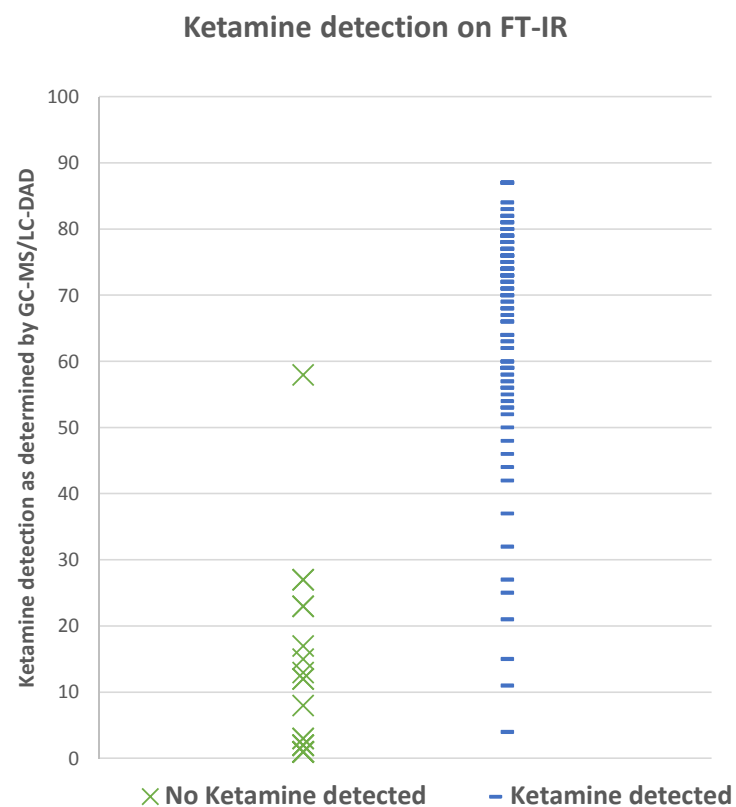
Results

Perks & Limitations

Future plans

# Which substances did the FT-IR miss? (optimal)

Every hit in single hit analysis or mix analysis counts as “detected”



- **Ketamine often missed by the FT-IR analysis**

- Bad reference spectrum in library?
- Mixtures
- “Bad luck”
- Drawback of method

DIMS

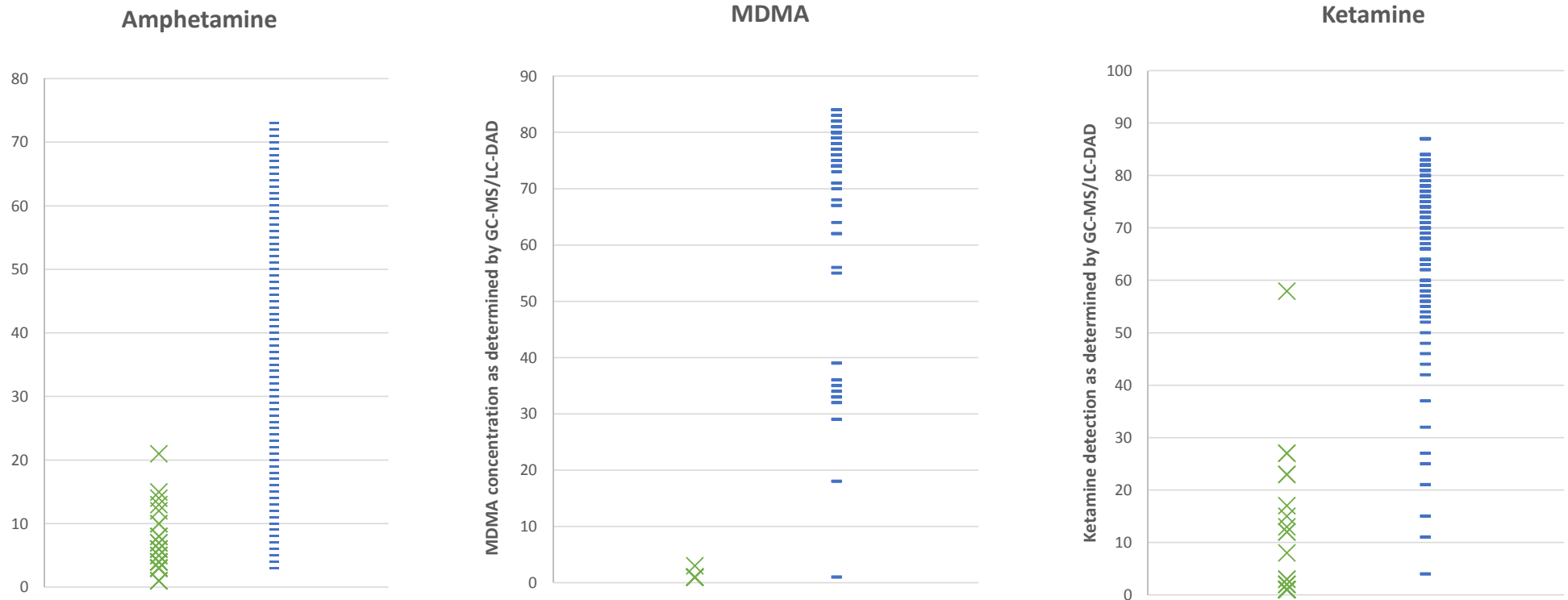
FT-IR

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Perks &amp; Limitations

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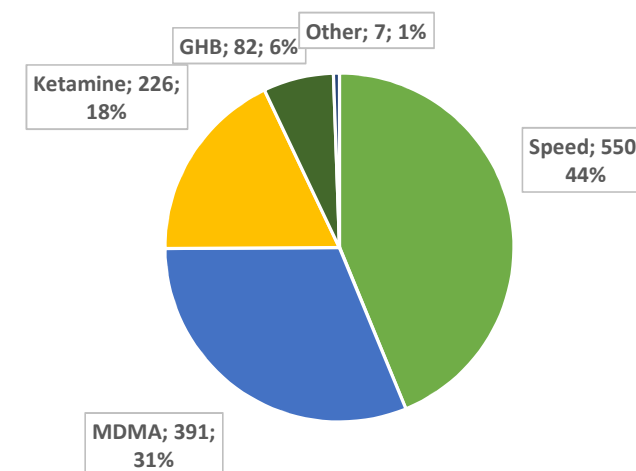
# Which substances did the FT-IR miss? (optimal)



**Big differences in Limit of detection between different substances and between different mixtures!**

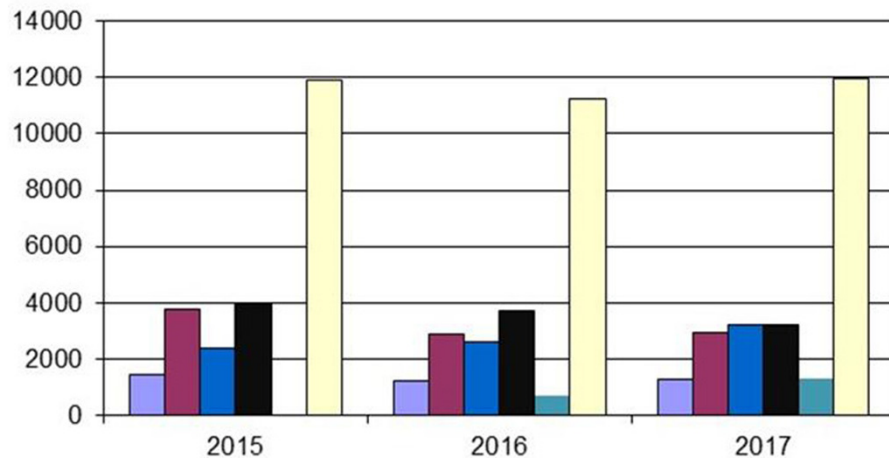
# Perks & Limitations

- **Perks**
  - Possible to have 100% true positives
  - Solid detection of main component
  - Semi quantification
  - Sometimes detection of secondary and tertiary components
- **Limitations**
  - Sometimes detection of secondary and tertiary components
  - Big differences in LOD between substances
  - Adulterations!
    - Prime example: Levamisole (cocaine)
  - Fentanyl....
- **Working experience at DIMS**
  - Very useful supplementary method
  - Shortcomings are covered by GC-MS/LC-DAD possibilities




# Future plans

- **Continue to develop new methods**
  - Software (OPUS) could be a lot better
  - Detection could be improved tremendously using different approaches
  - Time/gain



RESEARCH ARTICLE

### Rapid classification and quantification of cocaine in seized powders with ATR-FTIR and chemometrics

Joy Eliaerts , Pierre Dardenne, Natalie Meert, Filip Van Durme, Nele Samyn, Koen Janssens, Karolien De Wael

First published: 15 December 2016 | <https://doi.org/10.1002/dta.2149> | Cited by: 2

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#### Abstract

Traditionally, fast screening for the presence of cocaine in unknown powders is performed by means of colour tests. The major drawbacks of these tests are subjective colour evaluation depending on the operator ('50 shades of blue') and a lack of selectivity. An alternative fast screening technique is Fourier Transform InfraRed (FTIR) spectrometry. This technique provides spectra that are difficult to interpret without specialized expertise and shows a lack of sensitivity for the detection of cocaine in mixtures. To overcome these limitations, a portable FTIR spectrometer using Attenuated Total Reflectance (ATR) sampling was combined with a multivariate technique, called

DIMS

FT-IR

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**Future plans**