UNIVERSITY OF AMSTERDAM

FORENSIC RESEARCH PROJECT

RESEARCH PROJECT

Title	: Prediction of hand-held spectroscopy performance on screening for drugs of abuse using a master spectral database
Keywords	:
Forensic Expertise Area	: Rapid screening, illicit substances
Department	: Wageningen University and Research
Institute/Company	: Wageningen Food Safety Research
City	: Wageningen
Country	: The Netherlands
Supervisor	: Yannick Weesepoel and Martin Alewijn
Email address	: yannick.weesepoel@wur.nl; martin.alewijn@wur.nl
Telephone number	: 0317 480356
UVA Examiner	: Arian van Asten
UVA Coordinator	: Arian van Asten

SHORT DESCRIPTION

Small spectroscopy handheld devices (like near-infrared spectrometers) have the potential to be universally applicable for the on-site screening of (list 1) drugs of abuse and fraudulent foods. Currently the market is being flooded with many different types of such handhelds with different specifications (i.e. spectral range, spectral resolution, type of detector, type of illumination). Therefore, the capability of a specific hand-held for screening for a certain substances or fraudulent product is *a priori* unknown. This makes it difficult and potentially labour intensive to make an educated choice for a (universally applicable) handheld. In order to circumvent this problem, prior knowledge on the potential performance of a handheld would facilitate the choice of hardware. One way to do this is to record spectral information of illicit substances using a broad-spectrum high-end device. Using the broad-spectrum information and the specifications of the hand-held, a prospectus can be made on the performance of the handheld.

However, most drugs of abuse and fraudulent products are not found in their chemically pure form. Illicit substances like cocaine, MDMA etc. have been cut with (a mixture of) substances.[1] Also, when looking to designer drugs, many structural isomers and new substances are being found continuously of which some are forbidden and other are legal (i.e. 2-FA, 3-FA and 4-FA). For most new designer substances it is also unknown if they can be identified using high-resolution and/or lower resolution spectroscopics. For fraudulent foods matters are mostly even more complicated, as is for example in olive oil fraud. Here also different processing grades and geographic provenancing come into play, next to the illegal admixing of inferior products.[2]

Therefore, in this research project, we would like to explore (i) the transfer of 'master' high-resolution data to hand-held devices for newly seized drugs of abuse and fraudulent food products, and (ii) to model for hand-helds the minimal spectral ranges and interactions to do

a good job as a practical screening tool . We expect that quite advanced application of multivariate statistics will be involved in this project.

You will be working in the team of Authenticity and Nutrients of Wageningen Food Safety Research. The team has a long track record in applied chemometrics for food authentication using data from many types of analytical instruments. In the last years, we collaborate with UvA, NFI, Customs Laboratory, RIVM, CLCH and the National Police on implementation of chemometrics for the identification of illicit substances using cheap handheld spectroscopic devices.

REQUIRED/RECOMMENDED EXPERTISE

-Structured approach with large datasets
-Understanding of multivariate statistics
-Basic knowledge on spectroscopics and their application to illicit substances and products
-Experienced in using R or Python.

REFERENCES

1. Kranenburg, RF, Verduin, J, Weesepoel, Y, et al. Rapid and robust on-scene detection of cocaine in street samples using a handheld near-infrared spectrometer and machine learning algorithms. *Drug Test Anal*. 2020; 1–15. https://doi.org/10.1002/dta.2895

2. Yannick Weesepoel, Martin Alewijn, Michiel Wijtten, Judith Müller-Maatsch, Detecting food fraud in extra virgin olive oil using a prototype portable hyphenated photonics sensor, *Journal of AOAC INTERNATIONAL*, , qsaa099, https://doi.org/10.1093/jaoacint/qsaa099