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Updates on The In-Field Detection of New Psychoactive Substances

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Introduction: New Psychoactive Substances (NPS) have posed public health risks and numerous challenges that hinder their detection. Enhanced detection is key as an early warning system to accelerate alerts to stakeholders. The aim of this work is to showcase our research on the in-field prediction of emerging NPS. **Methods:** Raman spectroscopy coupled with chemometrics, underpinned by *in-silico* studies were utilised for the detection of newly emerging NPS internet products. **Results:** In-Silico studies were performed and 53 NPS were selected as representatives of the chemical scaffolds of 478 NPS (“calibration” sample set) to generate a Principal Component Analysis (PCA) model. The model was validated using reference “validation” and “test” NPS. Another model was developed by adding common adulterants to the “calibration” set. The latter was challenged by NPS internet products with variable purity using both projection PCA and Soft-Independent-Modelling-of-Class-Analogy (SIMCA). Both models were then transferred on a handheld system to test model transferability in the field. NPS references projected onto a PCA model derived from a handheld Raman database comprising ‘representative’ NPS resulted in the identification of 89% of NPS ($\lambda_{\text{ex}} = 1064\text{nm}$). NPS products projected onto a PCA model derived from a handheld Raman database comprising ‘representative’ NPS and adulterants discriminated between NPS products based on their purity profile. SIMCA allowed a supervised pattern recognition to confirm the proximity of the “test” to the “calibration” set. **Conclusions:** A proof-of-concept, with the potential to accelerate the screening of emerging NPS, was developed and demonstrated its success in the in-field detection of NPS products.