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Rapid desorption and analysis for illicit drugs and chemical profiling of fingerprints by SICRIT ion source

Ciara Conway[1,2] | Markus Weber[2] | Allison Ferranti[2] | Jan-Christoph Wolf[2] | Christoph Haisch[1]

[1]Department of Analytical Chemistry and Water Chemistry, Technical University of Munich, Garching, Germany

[2]Plasmion GmbH, Augsburg, Germany

Correspondence
Christoph Haisch, Department of Analytical Chemistry and Water Chemistry, Technical University of Munich, Lichtenbergstraße 4, 85748 Garching, Germany.
Email: haisch@tum.de

Abstract

Forensic analysis can encompass a wide variety of analytes from biological samples including DNA, blood, serum, and fingerprints to synthetic samples like drugs and explosives. In order to analyze this variety, there are various sample preparation techniques, which can be time-consuming and require multiple analytical instruments. With recent advancements in ambient ionization mass spectrometry (MS), plasma-based dielectric barrier discharge ionization (DBDI) sources have demonstrated to cover a wide range of these analytes. The flow-through design of this source also allows for easy connection to a thermal desorption type of sample introduction. We present an in-house built thermal desorption device where the sample is introduced via a glass slide, which gets heated and transferred to the DBDI-MS with nitrogen for identification and semi-quantification. Using a glass slide as an inexpensive sampling device, detection limits as low as 20 pg for fentanyl are demonstrated. Additionally, a very precise (>96% accuracy) identification of persons based on the chemical profile of their fingerprints is possible, establishing a direct analytical link of the drug trace to the individual in one measurement. We compared the DAG, TAG, sterol, and (semi-)volatile region of the averaged fingerprint spectra over multiple days, showing the best model accuracy for identification based on the DAG region. The combination of thermal desorption and DBDI-MS minimized sample preparation, leading to an ultrasensitive and rapid analysis of illicit drug traces and the identification of underlying personas based on fingerprints.

KEYWORDS
DBDI, forensic, mass spectrometry, SICRIT, thermal desorption

1 | INTRODUCTION

The first and most renowned attribute for forensic identification of a person is their fingerprint. The unique pattern of the ridges on a person's finger can even be used to differentiate siblings and twins.[1] They are individual traces left behind by every one of us simply by touching a surface. Therefore, fingerprints are the commonly accepted identifier for border control or police investigations.

Despite its already unique pattern, much more information is hidden in fingerprints than typically used in forensic investigations.[2]

Since we carry and deposit chemical traces of objects, liquids, and other materials that our fingers come in contact with, the chemical composition of a deposited fingerprint can give further significant forensic information. These traces may contain skin care product residues, or any other chemical an individual has come in contact with, particularly illicit substances, such as narcotics, drugs, and explosives. However, even more information can be gained from a suspect due to each person having an individual metabolism and microbiome on their skin.[2] The chemicals secreted within a fingerprint's "fatty" trace contain highly specific chemical information on the person. This was observed in people using illicit drugs, as well as being treated for drug addiction, where picogram to nanogram traces of drugs or their metabolites were detected in the chemical composition of their fingerprints.[3] This chemical makeup may identify a person, even if the fingerprint pattern has been smeared or is incomplete. Previous works suggest that differentiation between different sexes, ethnicities, and habits, like drug abuse, is possible based on fingerprint composition.[4–7]

A recent review on chemical fingerprint analysis stated that 62% of the analysis methods used in the investigated literature, covering 2008–2020, used mass spectrometry (MS) or MS coupled to chromatography.[8] Besides standard methods, such as matrix-assisted laser desorption (MALDI) or liquid chromatography (LC) MS, a lot of ambient ionization methods have also been applied for the direct analysis of forensic traces and fingerprints.[3,9–11] These methods follow two different directions: (A) chemical imaging of fingerprints and investigation of the chemical composition changes, and (B) fast trace detection of drugs and explosive residues with minimal to no sample preparation. Of the two most known techniques, desorption electrospray ionization (DESI)[5] is mainly used for imaging purposes and can be used for illicit drug detection as well.[12] In contrast, direct analysis in real-time (DART) mainly focuses on fast trace screening. For example, DART has been successfully applied to determine traces of explosives and drugs in fingerprints down to the ng level.[13] Similar reports exist on other ambient ionization techniques like low-temperature plasma (LTP),[14,15] paper spray ionization (PSI),[16] or laser ablation direct analysis (LADI) in real-time imaging.[17] Techniques such as PSI have also been successful in the identification explosives within biological fluids.[18,19] Additionally, these techniques, PSI and DART, have been used to determine gunshot residues from both biological and non-biological samples, where DART was used to determine the difference between the gunshot residues of commercially manufactured guns versus 3D printed guns.[20,21] Whereas those reports mainly focus on the trace "contaminants" in fingerprints, the chemical composition of the endogenous matrix was rarely studied using direct ambient MS since it is a very complex mixture of amino acids, hydrocarbons, sterols, and so on. One approach was undertaken by Cho et al.[22] They used direct sampling and mapping of unsaturated hydrocarbons and non-polar lipids using a swab and TD-ESI MS approach. They investigated the distribution of these components over a single human body. Zhou et al.[7] applied DESI imaging and machine learning to differentiate fingerprints of different persons' gender and ethnicity.

A flow-through dielectric barrier discharge ionization (DBDI) source[23] combined with MS has demonstrated improvements in the application for detection of chemical warfare agents by using its soft ionization to keep molecules intact with a dominant parent ion.[24] The source has further advantages as a field deployable device as it operates in room air without any other consumables. Combining this technique with simple sample preparation techniques such as solid phase microextraction (SPME) has been used for the spatial distribution analysis of illicit drugs in mice.[25] Furthermore, SPME was used by Mirabelli et al.[26] for the ultra-trace (fg level) detection of illicit drugs in beverages, artificial urine, and plasma. The same author also reported the identification of (condom-) lubricant fingerprints for sexual assault cases, using DESI imaging.[27] Overall, these techniques are compatible with DBDI-MS, as it requires volatile samples, which is accomplished by the thermal desorption of analytes from the SPME fiber. Therefore, no matrix cleanup steps, such as protein precipitation or solid phase extraction, are required to treat the sample.

The current study now employs a simple thermal desorption device for glass slides with the DBDI source, mentioned above, to eliminate the need for long extraction times and enable high throughput screening (less than 2 min per sample). Besides the targeted screening and LOD determination for drugs in fingerprints, high-resolution MS spectra of fingerprints of different individuals on different days were recorded. A chemometric analysis is performed on the data to investigate the hypothesis of a "chemical fingerprint" for person identification. The presented methodology is fast (less than 2 min), sensitive (pg LODs), robust, selective, and does not need complex sample pretreatment, suggesting a high potential for in-field usage, for example, at airports or other points of interest.

2 | EXPERIMENTAL SECTION

2.1 | Materials

Standards for heroin-d9, cocaine-d3, and fentanyl (100 μg mL^{-1} each) were purchased from Sigma Aldrich (St. Louis, Missouri, USA). The polar lipids standard was purchased at Avanti Polar Lipids Inc. (Birmingham, Alabama, USA). Triacylglyceride standard was obtained from NU-CHEK-Prep, Inc. (Elysian, Minnesota, USA). Compounds and concentrations of the lipid standards are described in the Supporting Information (Table S1). Microscope cover glasses (24 × 50 mm) were obtained from Paul Marienfeld GmbH & Co KG (Lauda-Königshofen, Germany). Acetonitrile (LC–MS grade, >99.95%) and methanol (LC–MS grade, >99.95%) were purchased from Carl Roth GmbH + Co. KG (Karlsruhe, Germany).

2.2 | Sample preparation

All standards and samples were prepared on microscope cover glasses. For the calibration series, dilutions of each drug standard were prepared in concentrations of 1000, 100, 10, and 2 ng mL^{-1} in

acetonitrile for heroin and cocaine and in methanol for fentanyl. Aliquots of 10 µL were pipetted onto a glass slide, leading to absolute amounts of 10,000, 1000, 100, and 20 pg, respectively. The same procedure was applied to slides with previously collected fingerprints to test these drugs spiked on a more complex matrix. Additionally, to assess analyte transfer via fingerprints, 20 ng each of fentanyl, cocaine, and heroin were spiked on a single glass slide, and fingerprints were then collected after touching those slides. The hands were thoroughly washed afterwards to minimize absorption through the skin. All measurements were performed in triplicates. Blank fingerprint measurements for comparison were repeated nine times.

Polar and triglyceride lipid standards were diluted one to ten in methanol, and 5 µL were pipetted onto glass slides and left to dry before measurement. Fingerprints were collected from eight individuals directly onto the glass slides and stored for up to 1 day at 5°C before analysis. Three replicate fingerprints were collected from each individual's left and right thumb. Collection of fingerprints was done on 2 days, 4 days apart, resulting in 6 to 12 samples of each individual (one person was only present for the first measurement day).

2.3 | Thermal desorption and ionization

Samples were desorbed with an in-house built thermal desorption device (see Figure 1) at a temperature of 300°C for 30 s. The desorption device was flushed with dry nitrogen (3 L min^{-1}) to ensure a stable and clean background. Due to the nitrogen flow, surrounding air is completely excluded from the measurement. Slides are manually introduced with the sample facing the ion source. Ionization of the desorbed sample was carried out by a SICRIT ionization source (Plasmion GmbH, Augsburg, Germany) with an amplitude of 1600 V and a frequency of 15 kHz. The source is based on a concentric dielectric barrier discharge. The details of source geometry and plasma chemistry have been described in previous publications.[28–30]

2.4 | MS

A high-resolution LTQ Orbitrap XL mass spectrometer (Thermo Scientific, San Jose, USA) was used for detection and quantification. The following parameters were used for the LTQ Orbitrap XL: capillary voltage 2.6 V; tube lens voltage 70 V; capillary temperature 275°C; mass window 75 to 1200 m/z; micro scans 1; maximum injection time 250 ms. Automatic gain control (AGC) was applied. The measurements were performed in full scan mode with profile-mode acquisition and positive polarity. A resolution of 30,000 (FWHM at 400 m/z) was applied.

2.5 | Data evaluation

Extracted ion chromatograms (EICs) with a 10 ppm window have been extracted and integrated with Xcalibur (Thermo Scientific, San Jose, USA) for the calibration curves. Linear regression and calculation of the LODs according to the 3σ method have been calculated in R (R version 4.2.2).

Lipidomic samples, standards, and fingerprints, collected from the Thermo-Orbitrap, were processed through an R-script and a Python machine learning pipeline. Raw spectra were centroided and converted to mzML with MSConvert,[31] and processed with PyOpenMS[32] (see Figure S1). A Zhang Fit baseline correction[33] and Savitzky–Golay smoothing algorithm, peak detection, and background subtraction

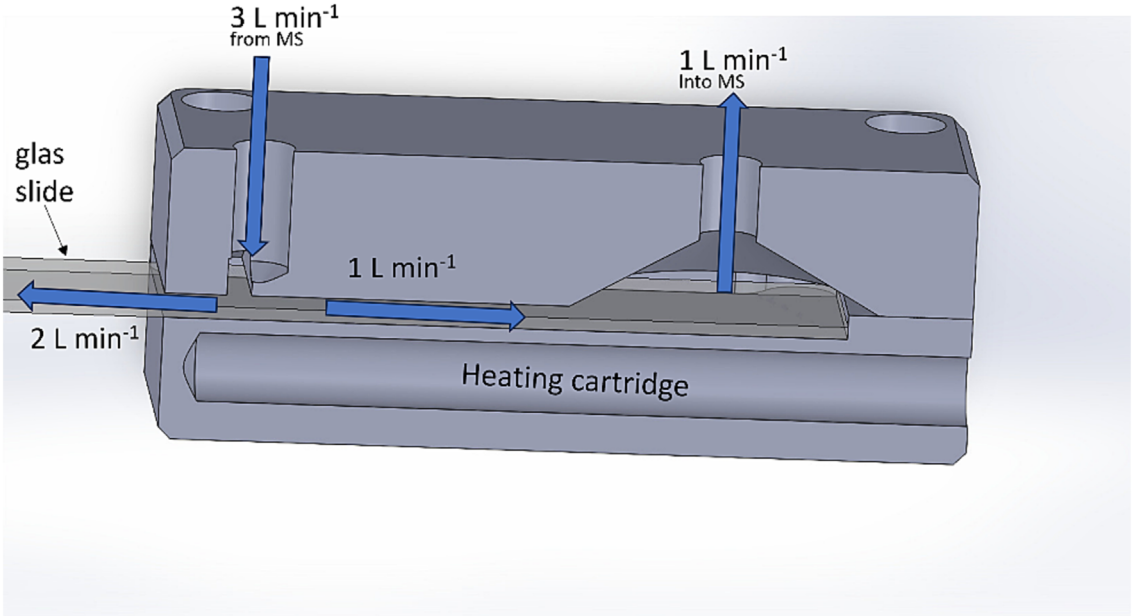

FIGURE 1 Cross section of the aluminum thermal desorption device with inserted glass slide. Arrows indicate gas flows coming from the MS interface flowing through the desorption device directly into the ion source and mass spectrometer.

were applied to the extracted MS1, averaged over a given retention time window. The cleaned MS1 peaks were exported as a feature table, with mz values as columns. To properly align the spectra across all samples, a virtual lock mass algorithm was applied to the feature table, merging redundant features with a 0.01 mz-value window shift, returning a reduced feature table. This aligned feature table was further cleaned by dismissing any feature missing from at least 90% of the samples. Furthermore, if a feature was not observed consistently within two thirds of the triplicate or sextuplicate samples collected, that feature would also be considered noise and discarded.

After an initial PCA to observe the separation of different individuals, a machine-learning pipeline was constructed to find an optimal model for this differentiation. The data was split 70:30 into a training and test set, where the sample separation was stratified and randomized. Due to the multi-class nature, the data had to be binarized. The sklearn Pipeline class was utilized to apply a series of dimension reduction methods and classifiers to the data to determine which model combination could best suit this type of data. First, a standard scalar was applied to the data, then a mixture of linear (PCA and SVD) and manifold learning (IsoMap and Locally Linear Embedding) dimension reductions were introduced to the machine learning pipeline. Dimension reduction methods were mapped to each classifier (Random Forest, K-Nearest Neighbor, Gaussian Process, Naïve Bayes, Decision Tree, and a Voting Ensemble method) with a range of potential parameters for each classifier. These constructed pipelines were introduced to a Leave-One-Out cross-validation grid search, providing the optimal classifier model for each combination based on the validation accuracy.

3 | RESULTS AND DISCUSSION

3.1 | Detection and identification of drugs

Unknown compounds were identified based on exact mass in the high-resolution mass spectrum. This was tested with three drugs (Fentanyl, Heroin, Cocaine) with absolute amounts of 20, 100, 1000, and 10,000 pg (for typical spectra; see Figure 2). Direct thermal desorption of samples was completed in only 2 min. All three compounds were ionized as protonated molecules.

The limit of detection for the pure substances was determined to be 4.5, 35, and 12 pg, respectively, for fentanyl, heroin, and cocaine on clean slides. The applicability of the thermal desorption device for trace amounts present in forensic samples, like fingerprints, was

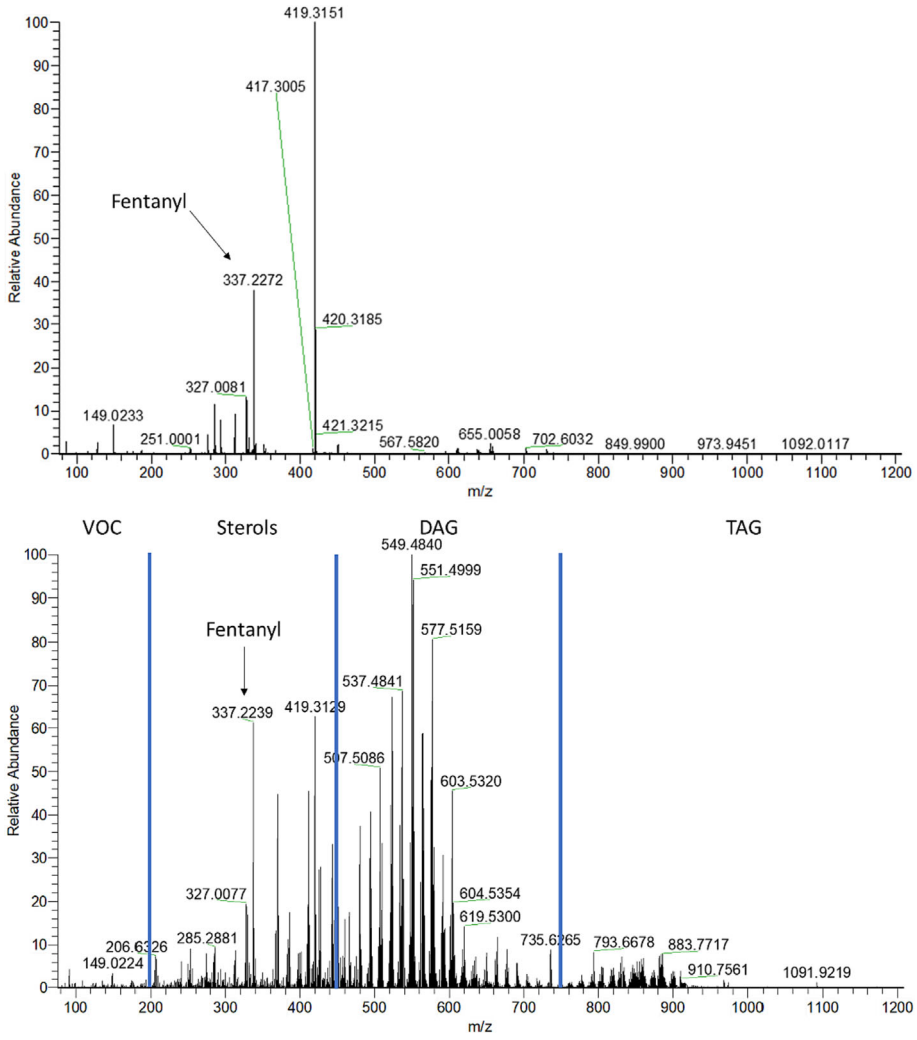

FIGURE 2 Comparison between spectra of 10 ng fentanyl on clean slide (top) and 10 ng fentanyl on slide with fingerprint (bottom). Different regions in the fingerprint are marked as volatile organic compounds (VOC), sterols, diacylglycerides (DAG), and triacylglycerides (TAG).

tested with spiked fingerprints equivalent to the pure substances (see Figure 3). LODs were in the same order of magnitude, with 54, 5, and 15 pg, respectively, for fentanyl, heroin, and cocaine; even with the heavy background consisting of lipids, amino acids, and other compounds present in the fingerprints. These values are in the range that can be expected to be found with a drug user, according to previous publications.[3] Due to manual sample introduction and relatively low scan rate of the Orbitrap, RSDs are relatively high with 10%, 11.7%, and 19.6% for 1 ng of pure fentanyl, heroin, and cocaine, and 51.6%, 14.9%, and 54.8% for 1 ng of each spiked onto fingerprints, respectively. Therefore, only qualitative or semi-quantitative measurements are possible. The identification is not limited to drugs but can also be applied to other compounds, such as lipids or explosives.

3.2 | Detection of drugs in fingerprints

The sensitivity is more than sufficient to detect a contact with even the smallest amounts of drugs. Figure 4 shows the difference between blank fingerprints and fingerprints after contact with 20 ng of the respective drugs on a logarithmic scale. Significant differences of multiple orders of magnitude have been observed for all drugs. The relatively large standard deviations are due to the inherent low reproducibility of substance transfer by touching a contaminated slide with one finger and then leaving a fingerprint on another slide.

3.3 | Identification of individuals based on fingerprints

During the measurements of contaminated fingerprints, differences between fingerprints of individual persons were observed. To further expand upon the forensic usage of the SICRIT technology coupled with a desorption device, we decided to investigate those differences further for the differentiation of persons based on the chemical profile of a fingerprint. This could be highly useful in the case of smeared fingerprints, which otherwise would be of no forensic value. Most signals observed in fingerprints could be identified as lipids. Based on this observation, a proof of concept measurement including two lipid standards was conducted to assess the suitability of the thermal desorption SICRIT setup for different lipid classes. The majority could be observed in high intensity (for details by compound class and EICs, see Figure S2). This proves that the SICRIT-desorption device is highly effective, even for compounds outside of the volatile range, with an excellent ion efficiency, allowing us to capture a complete profile of an individual's volatile and lipid fingerprint. As a first step for differentiating persons, principal component analysis (PCA) was applied to different parts of the fingerprint spectrum.

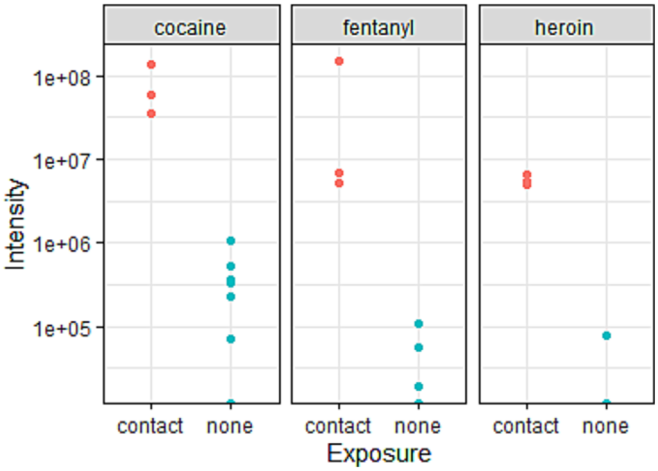

FIGURE 4 Comparison between non-contaminated and contaminated fingerprints after contact with 20 ng of the respective drug.

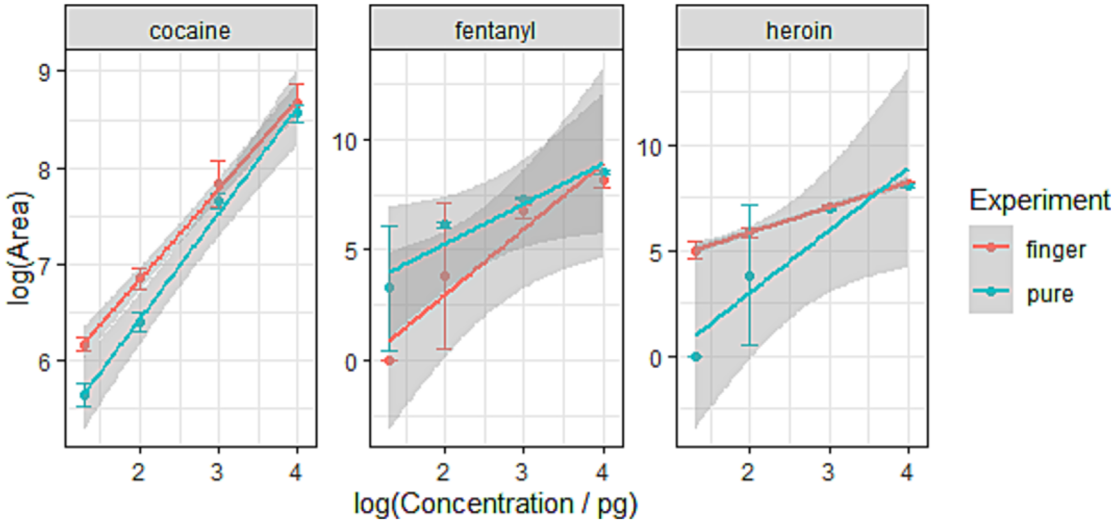

FIGURE 3 Calibration curves with 95% confidence intervals of cocaine, fentanyl, and heroin on a double logarithmic axis for pure samples and spiked fingerprints.

As an initial step, PCA plots were constructed from principal components 1 and 2 (see Figure 5), which show separation between some fingerprints of different individuals, even over multiple days. As a next step, a machine learning pipeline was implemented for testing different combinations of preprocessing, dimension reduction, and classification algorithms with the respective tuning parameters for the whole fingerprint spectrum and the different regions. The results of the best models for individual regions are summarized in Table 1.

The highest accuracy could be achieved for the full spectrum and the diacylglyceride (DAG) region with 0.9615, respectively. The other regions lead individually to lower accuracies, decreasing from the sterol over the triacylglyceride (TAG) to the volatile region. This is expected because the volatile region is highly dependent on the compounds a subject touched previously. Figure 6 shows the respective receiver operating characteristic (ROC) curve and confusion matrix for the best model on the full spectrum.

This study shows that the differentiation of fingerprints of eight different persons based on chemical composition is possible with this ambient ionization technique, even with fingerprints from different days. The individual measurement takes only 2 min. Further investigation with more test subjects of various demographics and over longer times is necessary to find out if this technique is also suitable for a comparison of one fingerprint to a database of the general public, as it is routinely done with the physical fingerprint pattern. But even

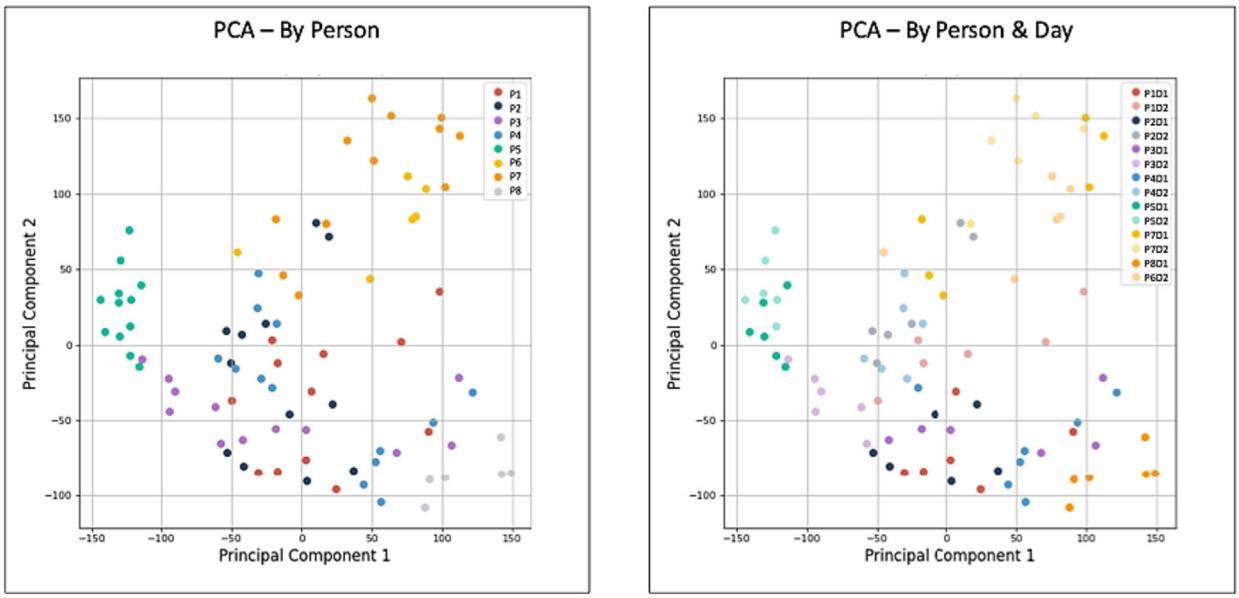

FIGURE 5 Plots of the first two principal components of the principal component analysis (PCA). Plot 1 shows PCA of the whole spectrum broken down to individual persons (left side) and persons and measurement days (right side).

TABLE 1 Summary of the models with the highest accuracy calculated on the test dataset for the full fingerprint spectrum and the individual regions.

Spectrum region	Best model	Accuracy	R^2	F1	Precision	Recall
All features	Dimension reduction: Truncated SVD (n_components = 20) Classifier: RandomForestClassifier (max_depth = 5)	0.9615	0.9918	0.9615	0.9615	0.9615
DAG region	Dimension reduction: Truncated SVD (n_ components = 20) Classifier: voting classifier	0.9615	0.9918	0.9615	0.9615	0.9615
Sterol region	Dimension reduction: LocallyLinearEmbedding (n_components = 16, n_neighbors = 16) Classifier: GaussianProcessClassifier (kernel = 1**2 * RBF [length_scale = 1])	0.9230	0.9836	0.9230	0.9230	0.9230
TAG region	Dimension reduction: LocallyLinearEmbedding(n_components = 16, n_neighbors = 16) Classifier: voting classifier	0.8461	0.9021	0.8461	0.8461	0.8461
Volatile region	Dimension reduction: LocallyLinearEmbedding (n_components = 16, n_neighbors = 16) Classifier: GaussianProcessClassifier (kernel = 1**2 * RBF [length_scale = 1])	0.7307	0.5841	0.7307	0.7307	0.7307

Abbreviations: DAG, diacylglyceride; TAG, triacylglyceride.

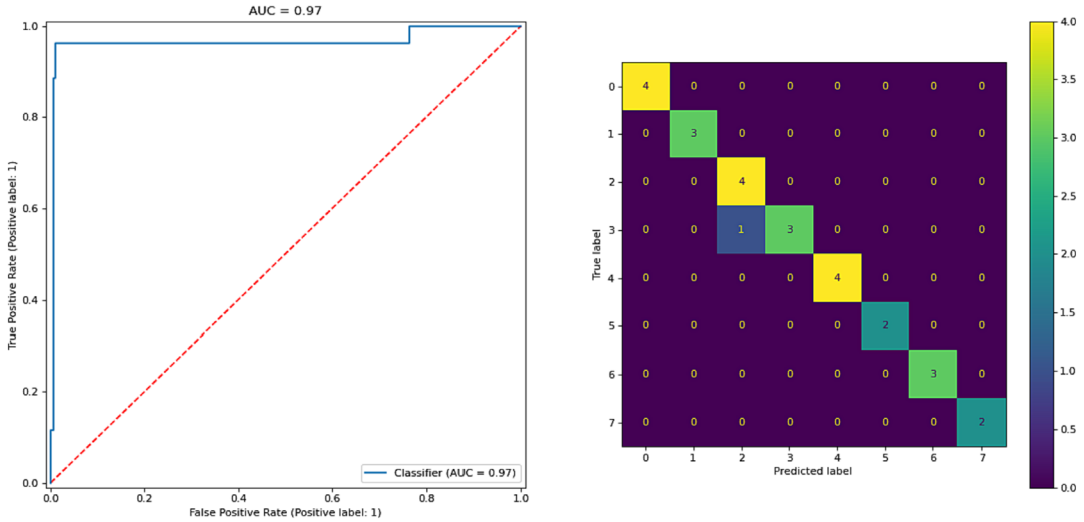

FIGURE 6 Receiver operating characteristic (ROC) curve and confusion matrix of the optimum model for the full spectrum (Truncated SVD (n_components = 20) and RandomForestClassifier (max_depth = 5)).

limited assignment of smeared fingerprints on a crime scene to one of few potential suspects can be a valuable tool for forensic application.

4 | CONCLUSION

This study presents a newly developed thermal desorption DBDI setup for fast and straightforward analysis of forensic samples. Identification of individual drugs can be done at low pg levels in only 2 min. This is also possible within complex matrices like fingerprints, allowing to confirm use or contact with drugs. Due to low power consumption and no need for additional (noble) gases, the method is well suited for transfer to mobile systems in the future. Utilizing high-resolution MS, fingerprints can not only be analyzed for specific compounds but also used to train models allowing to assign them to specific persons where fingerprints have been measured before. This is especially useful for smeared fingerprints that cannot be analyzed in a traditional manner. Overall, thermal desorption DBDI-MS provides fast, in-depth information about various forensic samples without complex sample preparation.

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ORCID

Markus Weber https://orcid.org/0000-0001-6465-0895
Jan-Christoph Wolf https://orcid.org/0009-0009-2394-1229

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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