Brief Report

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Brief Report

Multiplicity of Human Scent Signature in Identification of Persons by Computer-Based Olfactronics

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Abstract: This short report extends our previous paper "Multiplicity of human scent signature" and transfers canine identification to digital processing of data. The question is whether current GCxGC-MS technology and computer-based identification can perform identification as well as canines. This would objectify the identification of persons. Working with digital scent samples enables the use of multiple scent signatures for more exact identification. More differently constructed signatures during the identification process may represent the key point in identification of persons in olfactronics. Several types of scent signatures were considered in this article. The digital scent signatures were constructed based on the relative contents of the chemical compounds in the samples and relative ratios of compounds in the samples. Further on the signatures were made from the parts of the original samples fractioned by the volatility of compounds and by the relative abundance of the compounds in the samples. These results confirm the scent multiplicity phenomenon in digital scent samples. Using differently constructed signatures may be the key point in identification of persons using digital scent samples. This approach enables a transition from subjectivity to objectivity and a change from physical olfactory to olfactronic processing of digital scent samples.

Keywords: GCxGC-MS; forensic; olfactronic; scent signature; digital scent sample; identification of persons; chromatogram; multiplicity

1. Introduction

The multiplicity of scent signatures has been accepted as a fact by the scientific community [1,2]. This multiplicity was demonstrated on fractions of samples and identified by trained canines. It has been proven that canines do not only orient themselves according to certain specific compounds but have more options when identifying a person [1,3]. In other words, there must be more scent signatures in the scent samples.

The multiplicity of the scent signature can be viewed from several points of view. An interesting discussion is offered by the article [4], which studies the different scent signatures taken simultaneously from the breath and from the skin of the same persons.

The application of the olfactronic approach that uses computer-based identification is needed for the confirmation of the multiplicity of signatures, because it transfers the processing from the subjectivity of identification performed by canines to an objective computer-based software application [5,6]. The future use of trained canines in the identification of persons and in forensic work is addressed, for example, in the work [7]. The identification using canines can only be used as admissible evidence in court, not as conclusive proof [8].

The separation of the human scent into volatile and less volatile compounds opened the way to analyzing which compounds are important in identifying persons [9,2]. Reliance on volatile compounds led to an attempt to introduce the concept of a "human volatilome", when 1846 VOC (volatile organic compounds) compounds were identified [10]. Volatile compounds in the scent

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evaporate relatively quickly and are not usable in case of older samples. But the main disadvantage of volatile compounds is that they vary in their volatility and thus their mutual concentration ratios in the scent samples change over time [11]. Volatile compounds are likely to play an important role in determining the current state of a person, for example in the detection of a disease, they are promising for early and rapid detection of pathologies [12]. Less volatile compounds in human scent were thoroughly investigated in [1]. So far, 137 compounds have been identified, which are the best candidates for designation as primary compounds, that is, characteristic for a person and those by which it is possible to identify persons [13]. A relatively recent article [2] deals with the discussion of which substances are the most essential for identifying a person. Article concluded that rather than VOCs, these are moderately or less volatile compounds.

In the paper [1] the scent samples were taken from 11 volunteers who participated in identification and 20 other volunteers whose scent samples were used as controls. The samples from 11 volunteers were divided into 3 fractions according to volatility using the Agilent instrument (6890 GC/FID with an automatic Preparative Fraction Collector). A total of 33 fractional samples were prepared, 11 samples with high volatility, 11 with medium and 11 with low volatility. The division of the samples into fractions was done according to the 1D chromatogram record. The first fraction contained substances up to decanoic acid, the second fraction from decanoic acid up to squalene and the third fraction included compounds above squalene. This resulted in three fractions divided according to volatility – volatile, medium volatile and low volatile. These samples were tested by canines with three identification attempts. Six trained canines then identified fractions of the samples versus full samples. The total number of identifications by canines was 99. Success rate ranged from 36.7 to 83.3.

The subjectivity of canines manifests itself in the fact that each canine behaves differently during identification. Every canine has a distinct personality and they also cannot have identical training. The canines were of different ages – from three to seven years. Interestingly, the youngest had the second-best success in identifying samples, the oldest one the second worst [1].

2. Materials and Methods

Current experiments are trying to objectify the process of the identification of persons. Objective results must be unaffected by any subjectivity and must be reproducible and lead to the same results under the same conditions. Also, the division of the samples into fractions by means of computer procedure can be done so that there is an equal number of compounds in each fraction.

The samples used in this processing have been obtained from UCT Prague in 2022–2023. There were 13 volunteers, each of them provided 10 scent samples. 130 scent samples in total. The method of sampling the scent, extracting and measuring the scent samples has already been published by [14]. The samples were then processed on a GC×GC-MS chromatograph and subsequently evaluated by the ChromaTOF software (version 4.72.0.0) program with a signal/noise threshold of 100.

The files vary in size in terms of the number of compounds. An overview chart of the numbers is below in Figure 1.

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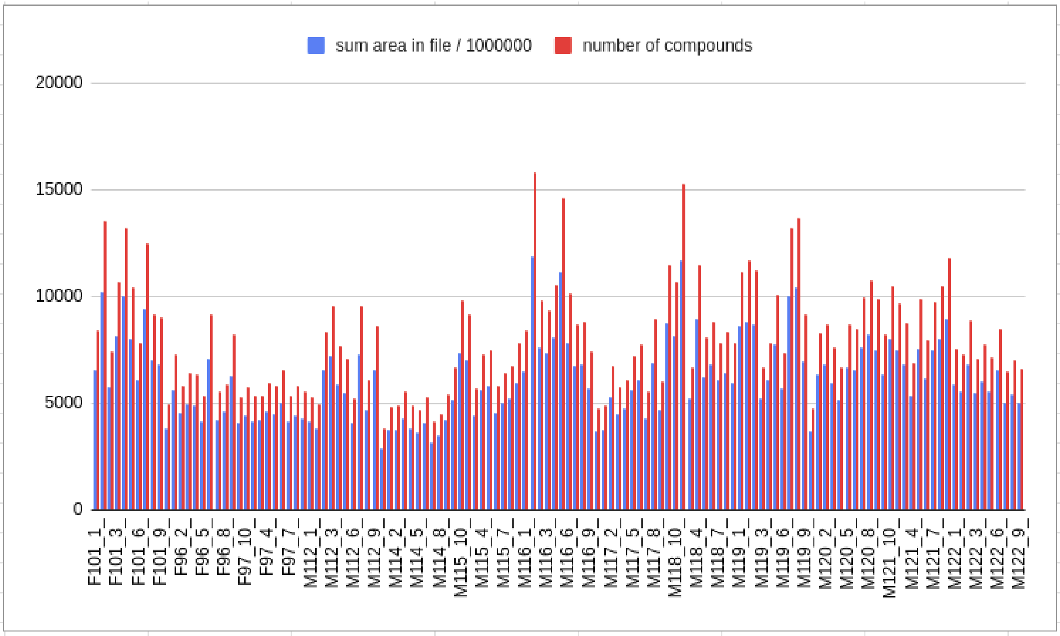

Figure 1. The different number of compounds in the samples.

The number of compounds in Figure.1 ranges from 3800 to almost 16000. This seems like a large difference; however, it means that many compounds are missing in the smaller samples. This is a problem because absent compounds cannot participate in the formation of the scent signatures. In practice, however, we see that scent samples themselves are not equally intense and it will certainly happen that the number of compounds must be different. We need only to ensure that some samples are not so weak that it would not be possible to identify signatures in fractions of the samples.

When using an olfactronic approach to processing data, we do not need to divide the data into physical fractions, but the division of compounds can be done by a procedure. The fractions of compounds can be prepared based on parameters. The scent samples were successively divided into three, four, five and six fractions so that each fraction had an equal number of compounds. The first group of divisions were made according to volatility, the two dimensions of the time were used to divide the compounds according to the distance based on the x and y axes, i.e. according to the calculated diagonal of the right triangle from the equation

$$z^2 = x^2 + y^2$$

Value of z is equal to $z = \sqrt{(x^2 + (60 * y)^2)}$

It was used because of the difference in dimensions, where the primary dimension is specified in units of seconds, whereas the secondary is in thousands of seconds. The primary time dimension in the graph ranges from 500 to about 3600 seconds, while secondary one from zero to ten seconds. (see Figure 2)

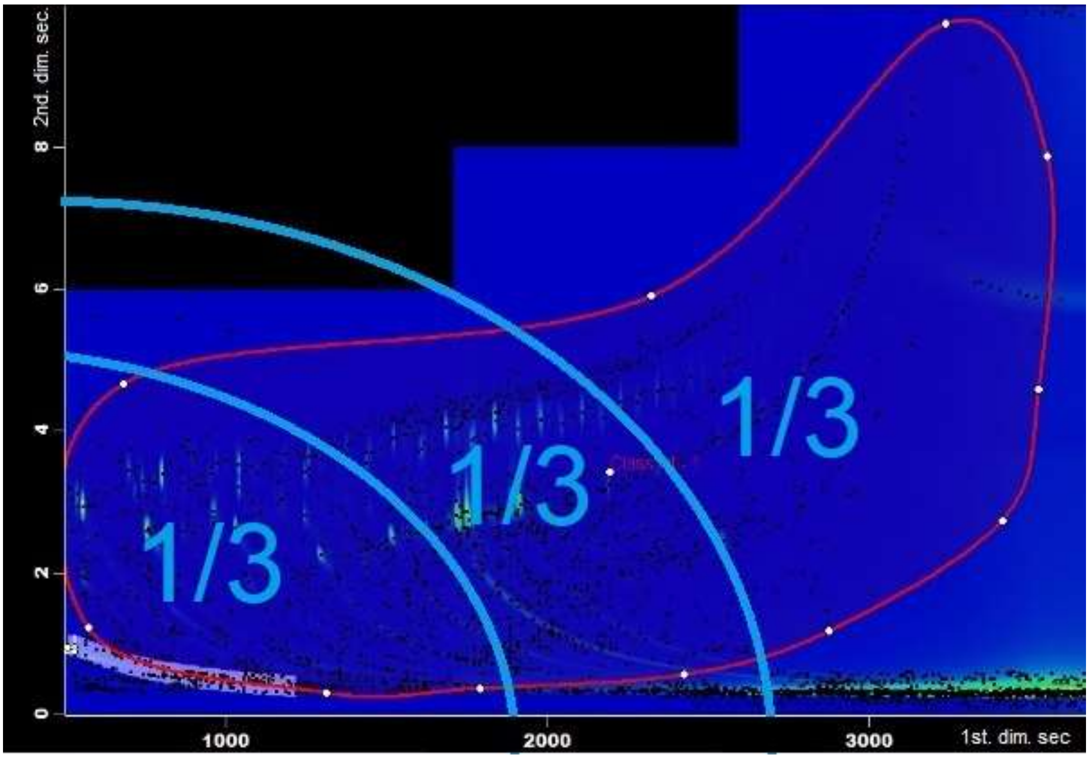

Figure 2. Division of the scent samples into three fractions according to the volatility of the scent compounds.

The second division into individual fractions divided the samples according to the field “area”. This corresponds to the amount of the compound in the sample. In the case of dividing the sample into three fractions, we get the first third of compounds that occur less frequently and have small peaks, then the second third of moderately occurring ones, and finally the third with the largest peaks, those that occur in the greatest quantity in the sample. Like the previous assumption with volatility, it would be assumed that those compounds that are more abundant in the sample could identify a person the best way. The opposite is shown, namely that the substances that occur in smaller quantities are more important for the identification. Those compounds that are in larger quantities in the samples are often in all the samples and also their mutual ratios differ, so they are not the primary compounds and are not significant for the identification of a person.

The processing of the identification of persons took place according to the article [15]. The two experiments are described here – the first division of the compounds according to volatility and in the second according to the content of the compounds in the samples. Both experiments took place in the same way – division into three, four, five and six separated fractions. Firstly, the test sample was selected from the person’s samples, then the scent signatures of the person were created from the other samples, and then the person’s own identification took place, i.e. the test samples compared to the prepared signatures. (see Figure 3).

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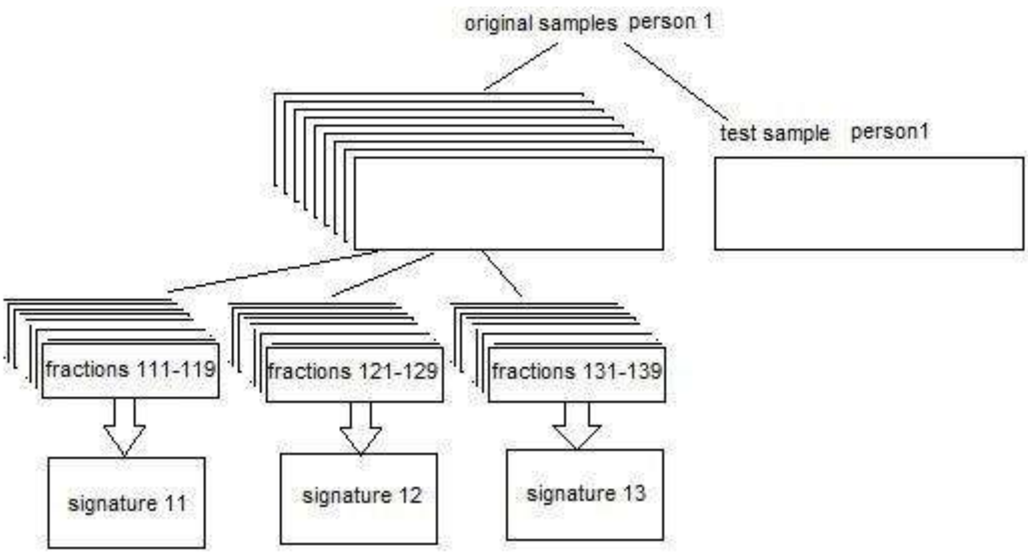

Figure 3. The creation of the signatures for every person and every fraction. Fraction 121 means that this fraction is for person 1, second fraction and first sample.

In each individual processing, all 130 samples were first imported into the database. Then the samples were divided into test samples and samples for creating personal signatures. Then the samples were divided into fractions according to parameters – how many fractions the sample is divided into, and which fraction of the sample is processed in this run. In the original article, there were 99 identifications. In this article, there were several thousand identifications that were performed sequentially with different test samples. This is much more than is possible with canines. The processing took place on a 64-core processor in eight simultaneous processes.

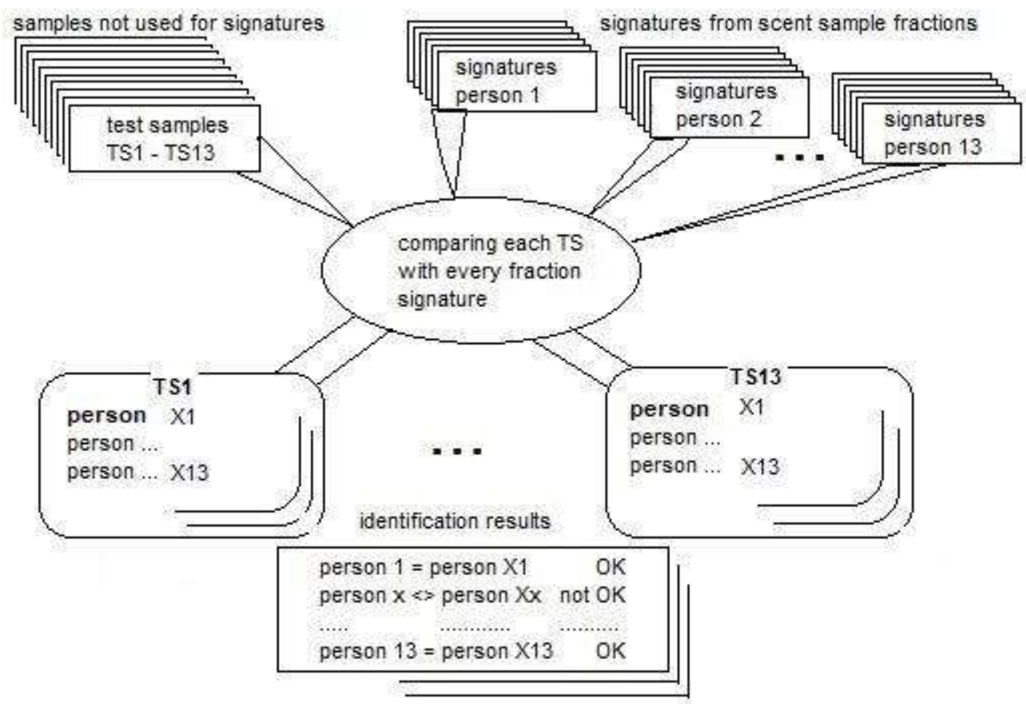

Figure 4. The comparison of test samples with signatures. Every test sample is compared with every pre-prepared signature. TS means test sample, Person X1... X13 are ids of person in result comparisons.

According to the conclusions from the article [15], the signatures were formed from eight samples and the number of pairs of compounds in the signatures was 8000. The summary results of

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the identifications based on abundance of compounds in samples are summarized in the following graphs.

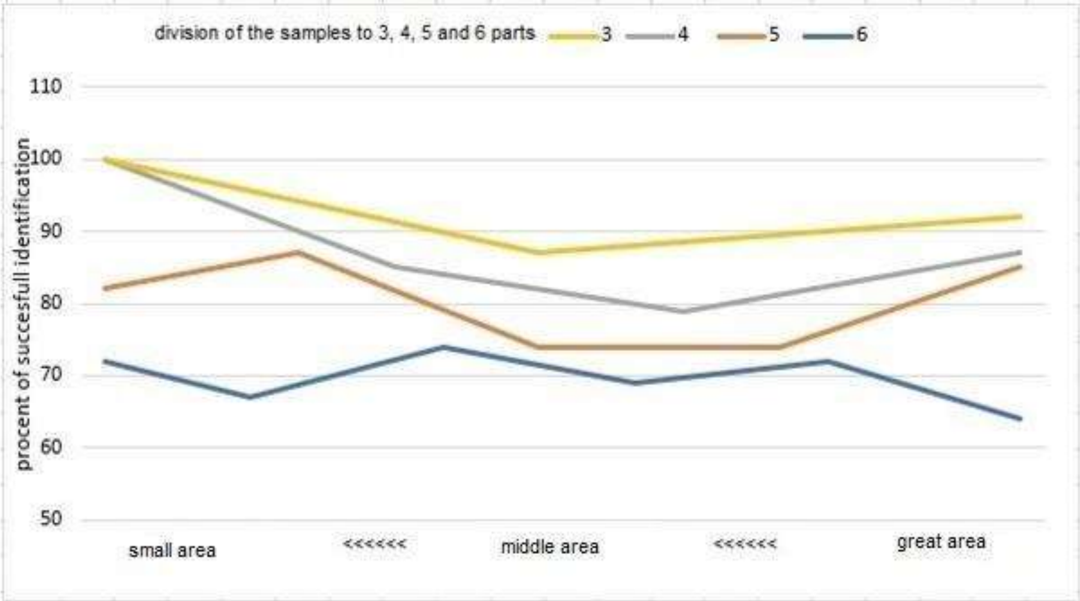

Figure 5. This graph shows four curves according to the number of fragments that the samples were divided into. The fragmentation is performed according to the area (quantity) in the samples.

The yellow curve in Figure 5 represents the division of the samples into three fractions, and the results show the percentage of identification success. Three fractions are present from left to right: the first with the compounds with the smallest peak area, the second fraction the middle size of peak area and the third on the right contains the compounds with the largest peak area value, i.e. those that occur the most in the samples. The surprising result demonstrates that those compounds that occur in the samples in the smallest amount are those that carry the most information for the identification of persons. So it is possible to identify persons based on them. This finding calls into question the method of selecting the most abundant compounds from samples and making an identification based on them. Almost one hundred percent success identification for the division of samples into three and four fractions (the yellow and gray lines in the graph) also proves the conclusions of the original article [1] about multiplicity of the scent signature in the scent sample.

The brown and blue lines show that dividing the samples into more fractions reduces the percentage of identification. The blue line shows the division of the samples into six fractions and the percentage of correct identification decreases to 70%.

The following graph (see Figure 6) shows the results of the identification of samples when divided into three, four, five and six fragments according to the volatility of the compounds.

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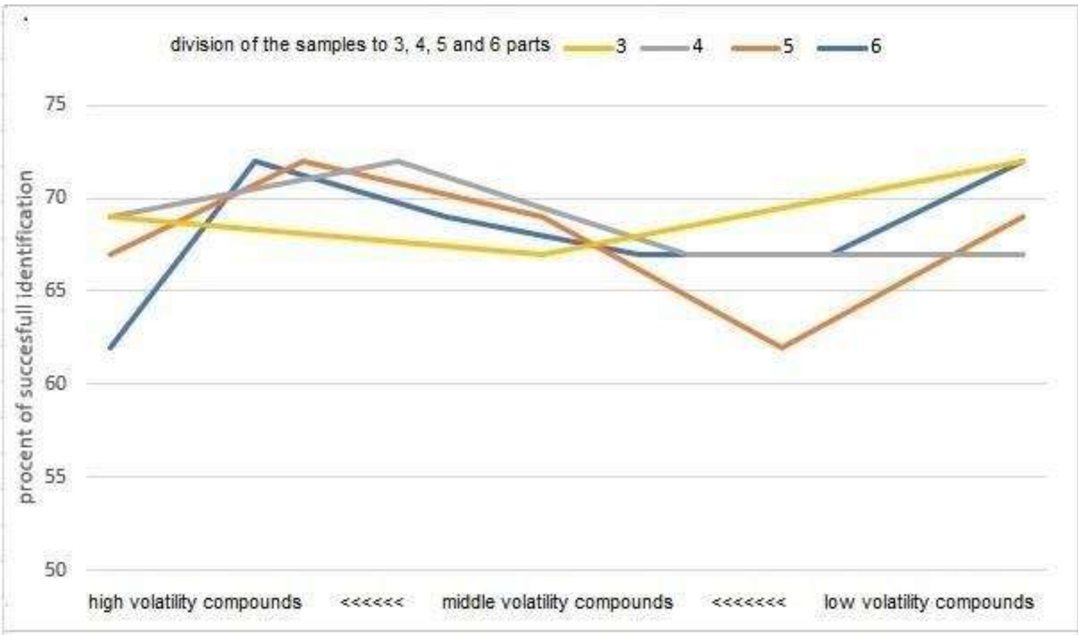

Figure 6. The graph that shows four curves according to the number of fragments than samples were divided into. The fragmentation is made according to the volatility of compounds in the samples.

The yellow line on Figure 6 represents the division of samples into three fractions, gray into four, brown into five and blue into six. From the very first look at the graph, it is clear that the identification took place with an overall lower efficiency of 62-72%. This result corresponds to the result in the original article, where the percentage of success was 58-85%. On the graph, we observe the increase in success identification for the fraction samples with low volatility compounds.

3. Results

Above all, the work confirmed the conclusions of the articles [1,16] that there are multiple scent signatures in one scent sample. Thus, it is possible to identify a person in certain cases by only fractions of the scent sample with the help of olfactronics. The possibility to identify people based on compounds with a small content in the sample was very clearly demonstrated.

Multiple signatures in a sample help to reach reliable, forensic identification of a person. For example, we can perform identification by the unfractioned sample and then by the fractions, where the compounds with the lowest area values are located. When identification of the same person is done according to both, the identification would be confirmed twice.

Thanks to olfactronics, it is possible to parameterize the processing of samples to signatures, adjust the parameters and even change the number of fractions of the samples. It is also possible to choose the method of the division of the samples.

4. Conclusions

The objective methods of computer-based olfactronic processing can be introduced in the scent identification of persons in forensic and police practice. The olfactory identification using police trained dogs can be extended by computer-based olfactronics. The olfactronic processing makes it possible to evaluate and store huge number of the digital scent signatures, whereas the identification credibility can be evaluated by means of chemometrics. Moreover, sophisticated databases can be created from these digital scent signatures.

The results have proven that with the use of GCxGC-MS chromatography and the digital processing of the scent samples it is possible to have even better results as trained canines. This objective olfactronic approach allows the identification of persons based on digital scent samples to be used in court cases as conclusive proof, not only as admissible evidence.

Author Contributions: LB analysis, programming, manuscript, ŠU: funding, outline ideas, manuscript check, UM: chromatography, manuscript check, publishing, All authors read and approved the final manuscript.

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Informed Consent Statement: Informed consent was obtained from all subjects involved in the study.

Data Availability Statement: Data used in the paper are available in Zenodo on the link: DOI: 10.5281/zenodo.10821605. Ten files for each of 13 persons, resulting in 130 files in experiments. Data are in TSV (tab separated values) text version.

Conflicts of Interest: The authors declare no conflicts of interest.

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