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PowerSorb® for forensic investigation of VOC traces: Application on perfume traces

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ABSTRACT

This study aims to assess the potential of PowerSorb®, a crime scene easy-to-use polydimethylsiloxane-based adsorbent, for the extraction of volatile organic compounds (VOCs) from olfactory (scent) traces. The PowerSorb®'s capacity for VOC collection is tested through increasingly complex extraction scenarios, using three commercial perfumes. Four scenarios were considered: (1) Direct analysis of liquid perfumes; (2) extraction of VOCs from liquid perfumes using PowerSorb®; (3) extraction of VOCs from polyester fabrics impregnated with perfume using PowerSorb®; and (4) extraction after cross-transfer between fabrics treated with different perfumes using PowerSorb®. Headspace Gas Chromatography coupled with a mass spectrometer (HS-GC/MS) has been used for the analysis. The results support that PowerSorb® does allow the adsorption and thermal desorption of VOCs. While measurement of uncertainties increases with the growing complexity of the transfer, PowerSorb® appears to be an efficient and easy-to-use tool for VOCs collection and the perfume's identification, when compared to more traditional sorbent phases, such as solid phase microextraction (SPME), which is hardly suitable for real-case scenarios. Olfactory traces remain challenging in cross-transfer scenarios, and further studies should be developed to assess the different perfume's dynamics (transfer, persistence, background, evaporation, and degradation).

1. Introduction

The Sydney Declaration defines traces as past remnants of presence or activity. They are the object of interest of forensic science [1]. Perfumes provide olfactory traces for forensic scientists. Olfactory traces are complex, since they include all the fragranced products (cosmetics, soaps, perfumes), human scent, and odorous environmental contaminants. Fragrance is a term used to describe an odorous compound or mixture. The olfactory traces are composed of volatile organic compounds (VOCs). This type of traces is highly dynamic, and its composition and behavior are not well known at the moment. The forensic interest in scent traces has been increasing over the years, with research on various odorous traces [2], perfumes [3–7], human scent [7–16], and the discrimination of human scent by tracker dogs [17–23]. Nevertheless, few of those studies have addressed the challenge of collecting such traces at the crime scene, except for sealing the support to send it to the laboratory, despite acknowledging the high dynamics of this kind of traces.

1.1. Challenges facing the collection of perfume traces

Many perfume types exist based on the alcohol fragrance mix concentration. The most popular types of perfume are listed below in Table 1.

To characterize the smell of fragrances through time, many types of so-called notes exist. For the first few minutes before evaporation, there are the top notes, which are the most volatile compounds. Then, there are the middle notes that stand on the skin for approximately 3 – 4 h before evaporation. The end notes are represented by the least volatile compounds, which give the depth of the scent and have persistence on the skin that lasts up to 5 – 8 h [24]. Due to the complexity of perfumes' composition and the increasing use of fragrances, researchers are currently trying to find ways to analyze and characterize the volatile organic compounds (VOCs) in perfumes. Still, they are also following the

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Table 1
Perfume type based on their fragrance fraction in alcohol.

Perfume type	Fragrance fraction in ethanol (%vol)
"Parfum"	15 – 30
"Eau de parfum"	8 – 15
"Eau de toilette"	4 – 15
"Eau de Cologne"	3 – 5

interactions with the human skin.

Currently, the chemical characterization and detection of olfactive compounds are made with gas chromatography coupled with mass spectrometry (GC/MS) [25]. Before the analysis, a good carrier of fragranced compounds is required for the sample preparation. A fragranced compound is volatile, which makes this step quite challenging. As well, to prevent the destruction of other traces, non-destructive collection methods are favored. In ideal circumstances, these collection methods should be extended to crime scene investigations.

Although numerous studies have been conducted on olfactory traces, only four studies by Simona Gherghel et al. have focused on the significance of fragrance traces, particularly those from perfumes, within a forensic context. They analyzed the transfer mechanism of perfumes [3] and developed an analytical method using solid phase microextraction (SPME) for the perfume's VOC [4]. Thanks to this validated method, Simona Gherghel et al. then studied the fragrance transfer [5] and persistence [6] on fabrics. All these works are conducted in a laboratory environment, which laid the foundations for a better understanding of the different perfume's dynamics (transfer, persistence, background, evaporation and degradation). Although, they fell short of addressing the challenge of an efficient and reproducible collector of such traces.

For now, Gherghel et al. used the SPME [4–6] to enable the collection and extraction of selective compounds within a complex matrix that conventional extraction methods (i.e. liquid-liquid extraction and solid-phase extraction) have difficulties with [26]. The SPME consists of a fiber coated with a specific polymer or a mixture of polymers to maximize the extraction of VOCs by using the interactions between the molecules and the polymer (hydrogen bond, dipole-dipole, Van der Waals, etc.) [26]. SPME fibers are also used in combination with chromatographic methods to lower the matrix effect, simplify the extraction, and develop faster analysis protocols. The use of SPME with the headspace (HS) method is also widely used to remove the potential matrix effect encountered in forensic contexts and to eliminate the sample preparation step before chemical analysis. The main default of these fibers is their low contact surface, which limits the fiber's extraction capacity [26]. To address this problem, the use of other adsorbent phases is under study, such as the PowerSorb®, which gives good extraction results in human odor profiles [8]. Considering the SPME limits, it would be interesting to evaluate the PowerSorb® extraction capacity specifically for the fragrance traces.

The PowerSorb® is a registered trademark deposited in 2017 by *Action Europe*® (Saugheim, France) [27]. This cylinder-shaped polymer is 20 mm long with a diameter of 2 mm (Fig. 1a). It simplifies the sampling method, since the polymer is conditioned under inert gas by the manufacturer. This allows exploiting the liquid, headspace (HS), direct, and passive sampling methods. The PowerSorb® may also be used during the extraction phase of the compounds, whether with the liquid-liquid extraction or with the thermal desorption methods [28]. In the literature, there are either the Sorbstar® or the Sorb-Star® that refers to the PowerSorb®. In fact, the three designations stand for the same polymer presented in Fig. 1a. The only difference comes from the manufacturer and its registered trademark. Between 2006 and 2016, there was a registered trademark called SORBSTAR® by *Applied Chemicals Handels-GmbH* (Wien, Austria) [29]. Since 2009, the Sorb-Star® registered trademark has been owned by *ENVEA GmbH* (Karlsfeld, Germany) [30]. The PowerSorb® has been used throughout this study. The PowerSorb® manufacturer [28] indicates that this product is suitable for several applications. These have been presented in the literature since 2017. It goes from the analysis of microplastics in water samples [31–33], the analysis of human scent with the possible application of the adsorbent polymer with tracker dogs [8–10], the analysis of polymers' degradation products [34,35] to the analysis of VOCs from human sweat to screen for breast cancer [36] which are all based on the thermal desorption method. Finally, the literature identifies one study that used the liquid-liquid extraction method with PowerSorb® to simulate food in the case of packaging degradation [37].

The focus of this exploratory study is on the use of PowerSorb® for perfume traces, as this study seeks to search for a simple method, potentially useful on-site, for the collection of scent traces, as close as possible to the crime scene, to minimize the high evidence dynamics of such traces. That collecting method would be used either as a complement or a substitute for the SPME fiber, as it is not always possible to bring such evidence to the laboratory.

Considering the literature described above, a method inspired by Gherghel et al. [4] has been used to assess the efficiency of PowerSorb® as a collector for the VOCs. In contrast to Gherghel et al. [4], who studied the behavior of target analytes to help their method's optimization, this exploratory study does not concentrate on specific VOCs, but on the capacity of the tested adsorbent to reliably collect the scent. The PowerSorb® is used for analyzing VOCs in increasingly uncontrolled environments through four different steps. As no standards were used to assess the molecule's nature, mass spectra (MS) are utilized to characterize specific VOCs within perfumes throughout the different steps. Thus, statistical results can be obtained from recurring VOCs' areas under the curve (AUC), allowing the assessment of the PowerSorb® and leading the discussion to the potential use of fragrance traces analysis within the forensic field.

2. Materials and methods

2.1. Materials

The present study focuses on a sorbent phase, presented above, called PowerSorb® (Action Europe, PT 70900). The supplier already conditions each PowerSorb® bar (Fig. 1a) in a 2 mL amber vial. Those

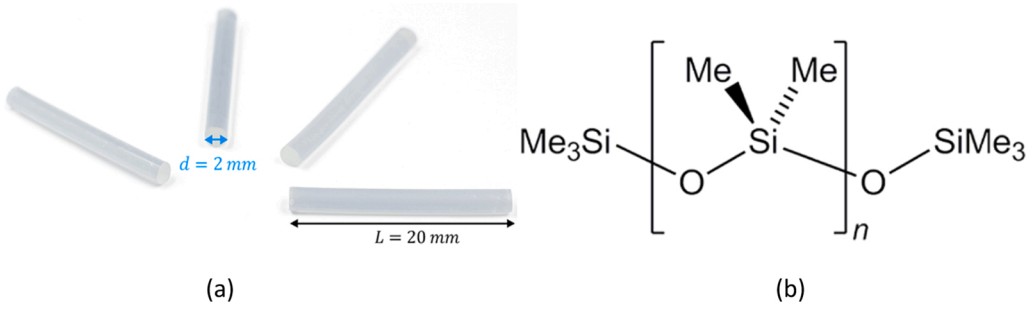

Fig. 1. (a) Representation of PowerSorb® [28] and (b) topological formula of PDMS [38].

sorbent bars are essentially made of polydimethylsiloxane (PDMS), as represented in Fig. 2b.

This study uses three commercial perfumes from different brands, two female "Eau de toilette" and one male "Eau de toilette", which were respectively called "A", "B", and "C". They were stored in the dark and at room temperature to minimize the perfume's degradation.

For the experiments, 100 % polyester fabric was chosen over cotton for perfume deposition due to its significantly lower matrix effects (i.e. hydrogen bonding and intermolecular forces) with the polar compounds [39]. The polyester pieces, each measuring 2 cm × 2 cm, and PowerSorb® bars were conditioned in sealed Arson bags (Forensics Source, PART ID1005339) well known and used in forensic science to prevent external VOCs contamination, but also as an adsorption chamber, exploiting their chemical properties: nylon bags are non-porous, preventing permeation of the VOCs and contaminant compounds as well as deterioration of the bag in long-term storage [40].

2.2. Sample preparation

2.2.1. Extraction and adsorption

The initial stage of this study involves extracting fragrance molecules, either in liquid perfumes or impregnated in fabric, to adsorb them onto the PowerSorb®.

Based on the article by Gherghel et al. [4], the optimal fragrances' extraction parameters from textiles are achieved by heating the sample to a temperature of 56 °C in an oven for one hour. These conditions contribute to the vaporization of the liquid matrix or the release of the VOCs contained in a fabric impregnated with 10 µL of "Eau de toilette". The different samples (see 2.4) were then prepared inside an Arson bag and sealed using a bag sealer (Philips Electronics, KB1000) before being placed into the oven.

2.2.2. Thermal desorption

Following the extraction comes the thermal desorption stage of the PowerSorb® for HS-GC/MS analysis. According to the manufacturer [28], the optimum desorption of PowerSorb® is achieved at 240 °C for 7 min. According to Cuzuel's study [8], optimum desorption occurs at 240 °C for 10 min. Considering the equipment available and the above recommendations, the thermal desorption took place in a GC/MS incubator (Agilent Technologies, 5977 A) at a temperature of 200 °C for 20 min. In terms of energy, 200 °C is relatively close to 240 °C, as both temperatures are about 4 $kJmol^{-1}$. This energy is sufficient to break Van der Waals forces, the predominant interactions between PowerSorb® and the perfume's molecules [41]. In line with the laws of thermodynamics, wherein desorption is dependent on the probability of interactions being dismantled effectively, the desorption time was doubled to avoid potential sources of errors during the extraction stage.

2.3. Chromatographic separation and detection

The instrumental parameters used are based on a method that has previously been validated for the analysis of VOCs using the GC/MS [4]. The capillary column chosen is of the ZB-5MSi type with a length of 30 m, a diameter of 0.25 mm, and a film thickness of 0.25 µm. This column is suitable for both low and high volatility compounds and is effective at temperatures between −60 °C and 370 °C [42].

The headspace of the vial containing the desorbed compounds from the PowerSorb® was sampled using a GC/MS 250µL automatic injection syringe MSH 02–00B at a temperature of 150 °C. The injection of samples from the final transfer study was carried out with a 250µL Hamilton™ Gastight SampleLock manual injection syringe at room temperature (~23 °C). The temperature of the injection port has been set at 250 °C. The injection process has three stages: a pre-injection delay of 500 ms, an injection with a speed of 500µL/s, and a post-injection delay of 500 ms. The injector is in split mode with a ratio of 20:1 in order to avoid overloading the column and potential damage. The GC oven temperatures were taken from Gherghel et al. [4] and are as follow: a temperature of 35 °C (held for 1 min) increased to 180 °C (held for 1 min) at a 5°C/min rate, and then to 300 °C (held for 2 min) with a 25°C/min gradient.

On leaving the column and arriving in the MS part, the compounds were ionized by electron impact at −70 eV in the source at 230 °C before reaching the quadrupole detector at a temperature of 150 °C. Data is acquired over a preset mass range from 50 to 450m/z.

2.4. Steps of the method

Four steps of the method have been carried out to assess the effectiveness of PowerSorb®'s analysis of VOCs from liquid perfume, perfume on a piece of fabric, and perfume transferred from another fabric. VOC extraction forms the basis of each step described below. The various steps are illustrated in Fig. 2.

The first and second steps used liquid perfume as a starting product, and have been triplicated for all three perfumes. Step 1 does not exploit the adsorbent polymer as the thermally condensed VOCs in an HS vial are directly analyzed. This first step is done to evaluate the potential of the analytical method for fragrances. Step 2, on the other hand, uses the PowerSorb® and goes through the stage of thermal extraction of the VOCs to adsorb them onto the PowerSorb®. The PowerSorb® is then thermally desorbed to allow analysis of the VOCs captured by the polymer. The second step reports on the direct effect of PowerSorb®. Hence, the second step assesses the adsorption in a closed environment,

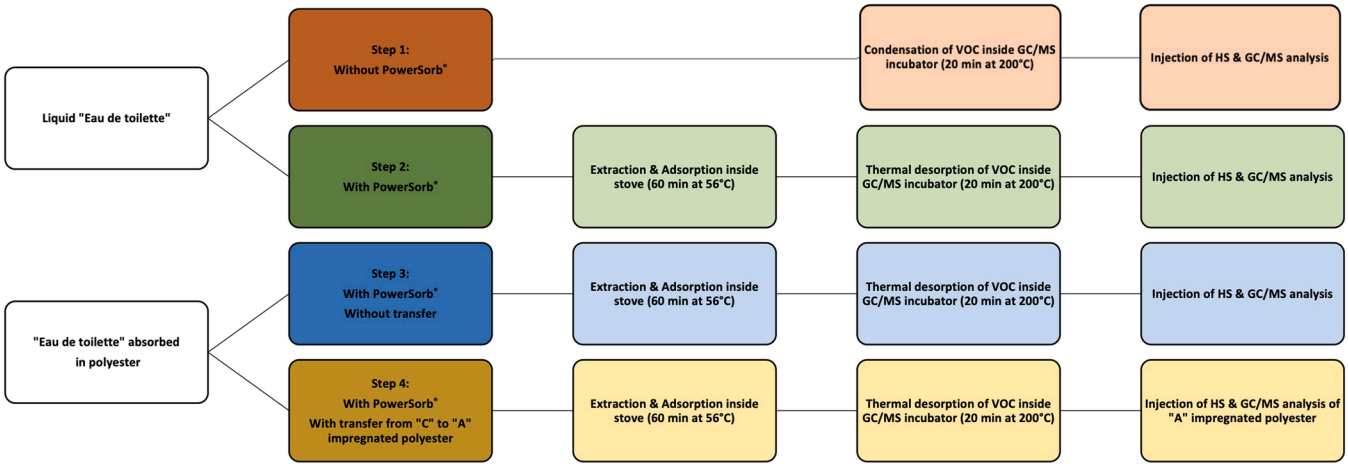

Fig. 2. Summary of the method's steps.

such as an Arson bag, and the desorption capability of the PowerSorb®.

Once the first two steps are deemed relevant in terms of reproducibility, the third and fourth steps evaluate the effectiveness of PowerSorb® on fragrance-impregnated fabrics. Step 3 is based on a perfume-impregnated fabric. Perfumes are vaporized onto the fabrics, and a delay of 2 min is implemented prior to extraction to allow the fragrances to impregnate the textile. For the third step, nine replications have been done for the “Eau de toilette A”, and three replications for the “Eau de toilette B” and “Eau de toilette C”. As this step is crucial for the study, “Eau de toilette A” has been analyzed in multiple replicates. Since it is not a standard, a higher number of replications was deemed necessary to assess the variation of this step effectively. Step 4 investigates a fabric initially impregnated with “Eau de toilette C”, which is then transferred onto a polyester piece that has been impregnated with “Eau de toilette A”. The latter has been analyzed using the GC/MS method presented above. The fourth step has been done once as a final exploratory illustration of an operational scenario. These last two steps of the method follow the same path. First, the VOCs from the impregnated or transferred fabric are thermally extracted in the oven and adsorbed onto the PowerSorb®. The PowerSorb® is then thermally desorbed in an HS vial before the GC/MS analysis.

3. Results

3.1. Qualitative analysis

The purpose of the qualitative analysis is to make a simple comparison between the quantity of VOCs detected for each "Eau de toilette" at each step of the method.

The number of compounds detected is an indicator of the method’s success, i.e. the possibility of detecting fragranced molecules contained in the perfumes following their thermal adsorption and desorption. The goal is then to detect as many compounds as possible from the reference, i.e. the perfume in its liquid form known as the perfume control. Three blanks were made: one with ambient air in the work environment, one with the polyester fabric and one with the PowerSorb® alone. Characteristic compounds from the blanks were subtracted from the analyses of "Eaux de toilette A, B and C". The subtraction was carried out and applied to the results of each step of the method. By analyzing the results in Fig. 3, it is possible to see many compounds for the “Eaux de toilette” studied in their liquid form (Step 1). Then, a drastic decrease in this number was observed when the PowerSorb® is integrated (Step 2). This is followed by a slight increase in the number of compounds detected when the method is used with PowerSorb® and impregnated polyester (Step 3).

The volatile organic compounds were observed systematically in each "Eau de toilette", which explains the absence of standard deviation in Fig. 3. In addition to the previous remarks, for each step, the number of VOCs detected is related to the “Eau de toilette C”. Finally, Step 1 extracts many compounds from the liquid perfume. Still, Step 3, with a non-negligible number of extracted compounds, remains promising if optimized.

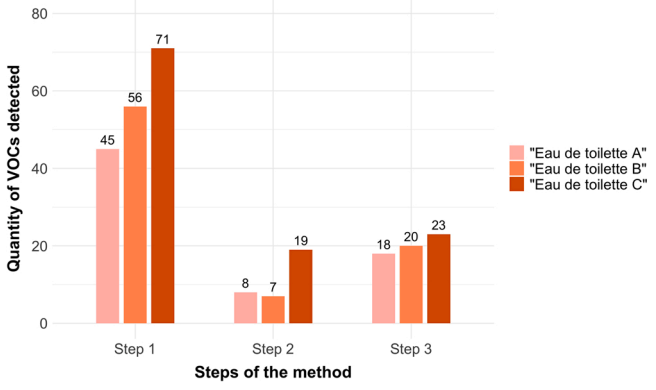

Fig. 3. Quantity of VOCs detected in each of the perfume’s replicate in terms of the different method’s steps.

3.2. Quantitative analysis

Repeatability of the retention time and mass spectrum allowed association of each molecule to a single numerical identifier throughout the various steps of analysis for the same “Eau de toilette” as shown in Tables 2 to 4. This identifier allows one to study the five VOCs that are always present in each step of the same perfume. The molecules’ nature is not explored further than their assessment through their corresponding mass spectrum; hence, no standards were used. Using the AUC for each of these compounds, which is linked to their concentration, coefficients of variation (CV) were calculated to evaluate the reproducibility of the method. Coefficient of variation, also known as relative standard deviation, is a robust parameter to compare results across different experiments, such as comparing the different steps as the complexity increases [43]. It is calculated with the following formula:

$$CV(\%) = \frac{Mean}{Standard\ diviation} x100$$

The following quantitative analysis expresses the results for the “Eau de toilette A”, but the same pattern has been observed for the B and C ones (see supplementary materials 1, 2, and 3).

To ensure the reproducibility of each step, it is recognized that the CV must be below 10 % [44]. Although for fragrance analysis of a small volume, higher CV could be tolerated [45]. In this case, it is reasonable to expect a low concentration for each VOC detected, considering there is 4–15 %vol of fragrance in the “Eaux de toilette” and a large number of fragrance compounds in this type of mixture. Hence, the “Horwitz Trumpet” [46] shows the increase of CV when the analyte’s concentration decreases. To go further in a forensic context, with the perfume’s dynamics (degradation, persistence, evaporation, background, and transfer), the expected concentration of VOCs would be even lower. Then, the analyst could accept higher intra-variability within replications from a single “Eau de toilette”.

Table 2 shows the results from the first step. According to the rule on the CV, this step is clearly reproducible with values between 0.36 % and 7.6 %.

Furthermore, Table 3 starts to support a lack of reproducibility with the VOC n°23, which is no longer the VOC with the lowest CV value. The CV values are dispersed for this step, but they stay in the acceptable region.

To complete the quantitative analysis, Table 4 shows that 14 % is the lowest CV value for Step 3, which could be considered as a lack of reproducibility and should be investigated. This step corresponds to the impregnated polyester with PowerSorb®.

3.3. Transfer analysis

This section focuses on Step 4, which is the transfer of a polyester impregnated with “Eau de toilette C” (Polyester 2) to another polyester impregnated with “Eau de toilette A” (Polyester 1). The results below come from the analytical analysis of the polyester with “Eau de toilette

Table 2
Statistical analysis regarding the “Eau de toilette A” from step 1 (n = 3).

VOCs	Average AUC ($\times 10^5$)	Coefficient of variation (%)
9	27	7.6
13	7.3	5.7
17	5.3	5.2
21	17	3.0
23	32	0.36

Table 3
Statistical analysis regarding the "Eau de toilette A" from step 2 (n = 3).

VOCs	Average AUC ($\times 10^5$)	Coefficient of variation (%)
9	8.6	3.7
13	0.62	5.6
17	2.2	0.89
21	0.39	5.5
23	0.46	12

Table 4
Statistical analysis regarding the "Eau de toilette A" from step 3 (n = 9).

VOCs	Average AUC ($\times 10^5$)	Coefficient of variation (%)
9	11	29
13	3.5	14
17	23	14
21	5.9	16
23	11	20

A" (Polyester 1). Fig. 4 below gives a visual summary of the transfer method.

The goal of Step 4 was to reproduce a simple forensic fragrance transfer scenario (without contamination and pollution) to assess the potential origin of the detected VOCs, whether it came from one specific perfume or both, considering the previous results. Due to the retention time and the mass spectrum, each detected VOC has been associated with its particular identifier number from the "Eau de toilette A", the "Eau de toilette C" or from both. Thus, the origin of the VOCs has been assessed, and the repartition is shown in Fig. 5.

The main goal of Step 4 is to assess the possibility of extracting and detecting VOCs from traces of the transferred "Eau de toilette". In addition, the discrimination between the transferred traces and those already impregnated on the original garment from another "Eau de toilette" may be done. A total of eighteen VOCs has been reported (see supplementary material 4). Fig. 5 illustrates that the most significant part of the extracted VOCs corresponds to the already impregnated fabric by the "Eau de toilette A". However, VOCs from traces of the transferred "Eau de toilette C" can also be isolated and analyzed.

4. Discussion

4.1. Qualitative analysis

The results in Fig. 3 show two crucial dimensions of the qualitative analysis. On one hand, it supports that the PowerSorb® is a good collector of fragrance compounds by adsorption. The thermal desorption of adsorbed VOCs can then be performed for subsequent analysis. This property is mainly due to the PDMS comprised within the PowerSorb® bars. This polymer is hydrophobic and porous and therefore enables electrostatic, Van der Waals, or hydrogen interactions [47]. The heat generated during the thermal desorption breaks down these interactions and induces the compounds' desorption. According to this, three parameters influence the number of VOCs detected: extraction type, temperature, and time.

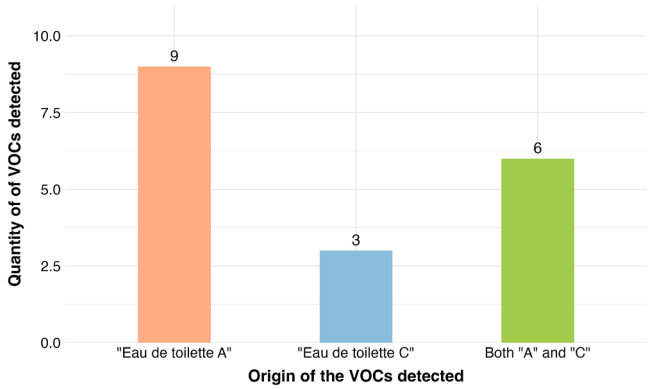

Fig. 5. Quantity of VOCs detected in terms of the perfume's origin from Step 4.

The extraction stage of this study was carried out using the passive diffusion of the VOCs under heat within an oven. No external devices, i.e. vacuum or pump, have been used to maximize the extraction yield of the VOCs. Moreover, increasing the extraction time promotes the adsorption of a greater number of compounds.

As for the extraction, the desorption temperature must be precisely adjusted to avoid premature desorption of the PowerSorb® or VOCs' degradation. Artifacts from the degradation of the VOCs will be visible during analysis if the temperature is too high [48]. This parameter should be high enough to desorb VOCs with the highest boiling point [8]. In terms of desorption time, it must be sufficient to allow the heaviest compound to desorb properly [8]. Overall, time and temperature must maximize extraction and desorption yields without damaging the odorous compounds of interest.

On the other hand, these empirical results (Fig. 3) are not in line with the initial expectation. A linear decrease was expected for the number of VOCs detected when the number of steps increases. This assumption comes from the fact that the more retention elements are added during the extraction stage, the smaller the number of VOCs detected will be. Thus, Step 1 should have the greatest number of compounds detected, where only the "Eau de toilette" is present (no retention element), and Step 3 should have the fewest number of compounds detected, due to the addition of two retention elements: PowerSorb® and polyester. Assumptions are formulated below to understand why the results shown in Fig. 3 are different.

For Step 1, the extraction of VOCs in a vial is made directly inside the GC/MS incubator at a temperature of 200 °C for 20 min. This step does not include the PowerSorb® since the headspace of the vial is analyzed. For Steps 2 and 3, the extraction process takes place in an oven for one hour at 56 °C and in a closed environment thanks to the Arson bag made of nylon. The PowerSorb® bar (in the original 1.5 mL vial) is placed in the Arson bag to adsorb the extracted VOCs. The Arson bag may retain the heat, lowering the temperature of the closed environment, where the samples from steps 2 and 3 are located. VOCs' evaporation could be affected, resulting in a lower quantity of VOCs adsorbed onto the PowerSorb®'s surface. The retention by the PowerSorb® and the closed environment's temperature may explain the drastic drop in the number of compounds detected between Step 1 and the two subsequent steps, but should be experimentally confirmed.

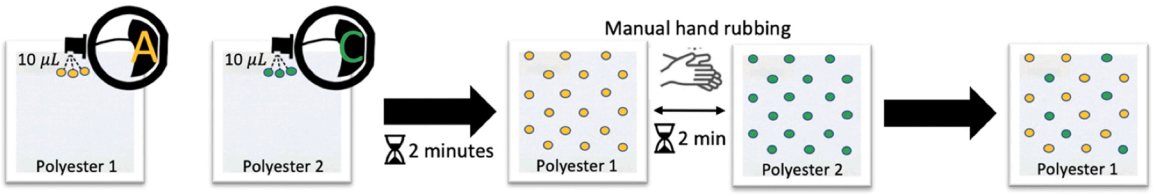

Fig. 4. Visual summary of the transfer method used in Step 4.

To explain the unexpected increase in the number of VOCs detected between steps 2 and 3, the difference in conditioning the «Eau de toilette» before extraction is considered. In Step 2, 10 µL of "Eau de toilette" is placed in a 20 mL glass vial, while in Step 3, droplets (10 µL) are dispersed directly on the polyester fabric for absorption. As the Arson bag may retain the heat, the glass vial does not reach a sufficient temperature to prevent condensation of the VOCs on the vial wall. Considering that VOCs have to leave the vial to reach the PowerSorb®, this increases the risk of condensation of the compounds found in the "Eau de toilette". Thus, Step 2 may have fewer compounds detected compared to Step 3, where compounds are initially free in the closed environment.

4.2. Quantitative analysis

Once it is known that the VOCs analysis is possible with PowerSorb® as a new VOCs collector, the reproducibility of the method can be assessed through quantitative analysis. To compare the first three steps of the method, the same five VOCs are analyzed in each step. The three main steps are part of a unique method of allowing repeatability to be assessed. This repeatability is evaluated at each step with variation coefficients to report the effect of increasing foreign elements (PowerSorb® and fabric) and, consequently, uncertainties. The analysis starts with Step 1, which represents the liquid form of the "Eau de toilette". The associated results are shown in Table 2. This step can be considered repeatable, as the 7.6 % CV value is significantly lower than the 10 % threshold [44].

Once the repeatability of Step 1 is confirmed, the analysis can proceed with Step 2 and the integration of PowerSorb® with the liquid form "Eau de toilette". Those results are presented in Table 3. CV values range from 0.86 % to 12 %, making them higher and more dispersed than those in Step 1. Although the CV of compound 23 (12 %) exceeds the threshold value of 10 % [44], this value is tolerated due to the small volume used [45]. Step 2 can therefore be considered as repeatable. However, the addition of PowerSorb® causes a slight increase in the results' dispersion, since adsorption of VOCs onto its surface is an additional uncertainty factor.

The impact of PowerSorb® is now assessed, and the Step 3 analysis focuses on the impact of impregnating "Eau de toilette" into a polyester fabric with PowerSorb® as a VOCs collector. The results in Table 4 show that the CV values range from 14 % to 29 %. They are much higher than 10 % [44], so this method's step is considered non-repeatable. This is due to the impregnation of "Eau de toilette" in polyester, adding another layer of uncertainty. It represents what is at the core of forensic science's observations, the trace. This Step 3 involves perfume's dynamics, such as the persistence, degradation and evaporation of the "Eau de toilette" on its substrate (polyester fabric). These dynamics effects are unknown and therefore contribute to the increased uncertainty and lack of repeatability.

In short, it can be seen that the coefficients of variation increase as the steps of the method evolve. This is particularly due to the addition of foreign elements, pushing the trace of "Eau de toilette" to become uncontrolled. The quantitative observations suggest that the method is repeatable. Outcomes discrepancy is caused by the very nature of the scent trace, its ontology. While in real life, this quality and the various contaminations cannot be controlled, it reminds forensic scientists that interpretation is at the core of their discipline, whatever the reliability of sensitive analytical methods, even at the source level [49,50].

4.3. Transfer analysis

It is now assessed that with the first three steps of the method, the PowerSorb® offers excellent reproducibility in terms of VOCs' extraction in a controlled environment. The contribution of the fourth step of the method allows the evaluation of the PowerSorb® on uncontrolled olfactory traces. As a matter of fact, the transfer involves all of the perfume's dynamics, such as the ability of VOCs to be transferred and the persistence of VOCs on both pieces of polyester, but also the background information on the initial fabric. These factors are not well known at the moment. The transfer step illustrates here the challenge of reality since forensic science has had to deal with a continuum of uncertainties daily when evaluating pieces of evidence that are degraded, contaminated and/or partial.

Initially, it was anticipated that the transfer results would show a majority of VOCs from "Eau de toilette A" and a minority from "Eau de toilette C". The results shown in Fig. 5 meet the previous expectations. Indeed, in a total of eighteen VOCs detected, it is possible to discriminate nine VOCs that came from the "Eau de toilette A" and three VOCs from the "Eau de toilette C". In addition, six other VOCs were detected in both "Eau de toilette A" and "Eau de toilette C". The discrimination of their source, whether they came from only one "Eau de toilette" or both, is impossible with the current analytical tools used. Even though we cannot assess their source, the four shared VOCs constitute a minority, and the discrimination worked for fourteen other VOCs.

Step 4 has been completed in only one replicate to establish a foundation for further research focused on PowerSorb® as a VOCs collector and the transfer analysis of fragrance. Indeed, the results show that the PowerSorb® can adsorb transferred VOCs, but cannot discriminate them from their original source while considering only the molecules' presence.

Overall, to lower CVs, it would be interesting to use the molecules' mass spectrum in an extracted ion chromatogram (EIC) mode to lower the background noise, which may help to lower intra-variability. There's also a need to develop a more specific analytical method for the PowerSorb®, as the current method used has had impacts on the accuracy of the results and its optimization for the PowerSorb® is essential. For the transfer analysis, it would also be interesting to see if the discrimination of VOCs from two "eaux de toilette" is possible using different analytical methods, such as the Isotope-Ratio Mass Spectrometry (IRMS), which could enable the discrimination of the same molecule that would have different origins.

4.4. Comparison with the Gherghel et al. approach [4]

Through this exploratory study of the perfume's traces, some differences have been noted between the obtained CV and those from Gherghel et al. [4]. For the fragrance's extraction from the polyester fabric (Step 3), coefficients of variation range from 15 % to 29 % in comparison to the 1.5 % obtained by Gherghel et al. [4] using a DVB/CAR/PDMS SPME fiber. Nevertheless, huge differences between Gherghel et al. [4] and this study could explain such discrepancies, which will be later investigated.

First, there is no use of internal standards within this study. The use of an internal standard is suggested when using a SPME [26], or any other sorbent phase, such as the Powersorb®, to reduce random variations from the analytical method, which could lower coefficients of variation. Despite this, the operational aspect must be considered, making the integration of internal standards demanding with textiles. Where would the internal standard solution be placed compared to the sorbent phase's position when enclosed with the textile? There is no certainty of the perfume's position on the textile, so the internal standard would need to be placed at the same position for each experiment. Considering this, this study evaluates the simplest extraction method for operational purposes.

Furthermore, the use of PowerSorb® is easier than the SPME. SPME requires dexterity and precision to realize the extraction and to prevent the fiber's breakage, which can be pretty expensive. On the other hand, PowerSorb® is handled easily and could eventually be brought directly to crime scenes by field practitioners (SOCOs and CSEs).

Subsequently, the details of the textile and the sorbent phase enclosure do not seem to be mentioned in Gherghel et al. [4], compared to this study. However, for operational purposes, Arson bags are used, in this study, during the extraction stage with the sorbent phase. These

plastic bags are utilized and have various applications within forensic science due to their impermeability to hydrophobic molecules, such as accelerants. One can argue that variations are related to the fragrance molecules' nature. These types of molecules are mostly polar and could have been lost by diffusion through the Arson bags during the extraction procedure. For the CV calculation, Gherghel et al. [4] used five compounds they thought were widely used in the perfume industry before their chemical analysis. A contrario, in this study, the five compounds considered for the CVs are selected after the chemical analysis. They are extracted at each step from every perfume. The selection of compounds before the perfume's analysis creates a potential bias within the results in favor of the SPME [4]. More precisely, the chosen molecules in Gherghel et al. [4] could be molecules known to be more stable through the thermal exposure of GC-MS analysis.

Furthermore, are the selected molecules more affected by the sorbent phase or the trace substrate, the polyester textile in this case, than the used molecules from this study? These different factors, determined at the start of this study, were not taken into account in Gherghel et al. [4] and could explain the CV difference between the two studies. Since this study is based on different compounds and higher CVs are obtained, could the molecules' nature influence the analysis of intra-variability and contribute to higher CVs?

More studies must be performed on these types of traces concerning the dynamics (background, transfer, persistence, evaporation and degradation) on different substrates and their interpretation. Gherghel et al. [5,6] are starting this discussion through the analysis of different parameters, such as the perfume's trace ageing and its transfer from one textile to another. They also used a mixture of five compounds, in addition to their internal standard, instead of an authentic perfume. This can impact results since perfumes are developed with various compounds other than fragrances, such as alcohol denaturant, anti-UV, anti-microbial, etc. [51]. These different compounds interact with each other, enabling a good quality perfume in which the volatility is controlled to give a scent for a certain time-lapse. In addition, different aspects need to be developed, such as the study of more complex scenarios. The textile used for the transfer study should already have a fragrance trace, which would complexify the discrimination of the original perfume. The dynamics of these traces, crucial for discriminating between two perfumes (victim and suspect), also necessitate the creation of the fourth step in this exploratory work.

Other interesting questions emerge and remain to be assessed, such as: Are the targeted compounds selective enough? Does their presence occur frequently, without the use of perfumes, in our daily activities? Is quantification, as performed in Gherghel et al. [4], required to have good discriminating power? These questions should be answered before the use of fragrance traces in real cases.

5. Conclusion

To summarize, this first exploratory research is developed to evaluate the PowerSorb® for fragrance compounds' extraction, as its characteristics may ensure proper VOC traces' collection and preservation directly from the crime scene. This study supports the ability of PowerSorb®, as a sorbent phase, to extract VOCs from commercial "Eaux de toilette". In a second step, the PowerSorb® enables the efficient thermal desorption of VOCs in a headspace phase for chromatographic analysis. Although the method is not optimized for this adsorbent phase, the current experimentation involved conducting fragrance trace analysis on textiles without contamination, as well as in a cross-transfer scenario. However, more research must be done to recommend the use of PowerSorb®. Future studies would develop a more specific extraction process for the PowerSorb®, or optimize its desorption to maximize the quantity of fragrance molecules and to lower intra-variability. Besides, studies about the nature of extracted fragrance compounds and their occurrence on fabrics would help interpret fragrance traces at source and activity levels [1].

CRediT authorship contribution statement

Elizabeth Audette: Writing – original draft, Visualization, Methodology, Investigation, Conceptualization. **Pier-Louis Dumont:** Writing – original draft, Visualization, Methodology, Conceptualization. **Frank Crispino:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Conceptualization.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.forsciint.2025.112605.

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