Non-invasive sorptive extraction for the separation of human skin surface chemicals using comprehensive gas chromatography coupled to time-of-flight mass spectrometry: a mosquito-host biting site investigation

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Running title: Human skin chemicals by GCxGC-TOFMS: a mosquito-host biting site investigation

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Article Related Abbreviations: GC×GC-TOFMS, comprehensive gas chromatography coupled to time-of-flight mass spectrometry; IS, internal standard; MeOH, methanol; PAHs, polycyclic aromatic hydrocarbons; PCA, principal component analysis; PDMS, polydimethylsiloxane; TD, thermal desorption; TIC, total ion chromatogram; VOCs, volatile organic compounds.

Keywords: comprehensive screening, skin volatiles, non-invasive sampling, passive sampler, mosquito semiochemicals

Abstract

Variation in inter-human attractiveness to mosquitoes, and the preference of mosquitoes to bite certain regions on the human host, are possible avenues for identifying lead compounds as potential mosquito attractants or repellents. We report a practical, non-invasive method for the separation and detection of skin surface chemical compounds and comparison of skin chemical profiles between the ankle and wrist skin surface area sampled over a five-day period of a human volunteer using comprehensive gas chromatography coupled to time-of-flight mass spectrometry. An in-house made polydimethylsiloxane passive sampler, worn as an anklet or a bracelet, was used to concentrate skin volatiles and semi-volatiles prior to thermal desorption directly in the GC. A novel method for the addition of an internal standard to sorptive samplers was introduced through solvent modification. This approach enabled a more reliable comparison of human skin surface chemical profiles. Compounds that were closely associated with the wrist included 6-methyl-1-heptanol, 3-(4-isopropylphenyl)-2-methylpropionaldehyde, 2-phenoxyethyl isobutyrate, and 2,4,6-trimethyl-pyridine. Conversely, compounds only detected on the ankle region included 2-butoxyethanol phosphate, 2-heptanone, and *p*-menthan-8-ol. In addition to known human skin compounds we report two compounds, carvone and (*E*)-2-decenal, not previously reported. Limits of detection ranged from 1 pg (carvone) to 362 pg (indole).

3.1. Introduction

The World Health Organisation (WHO) estimated that 228 million cases of malaria occurred worldwide in 2018 with most of the cases (93%) diagnosed in the African Region [1]. Vector control strategies such as indoor residual spraying (IRS) and long-lasting insecticidal net (LLIN) programmes have played a crucial part in the reduction of malaria cases between 2002 and 2017 [2-4]. There are two main problems affecting the future use of LLINs and IRS: firstly, these strategies used alone or combined will not eradicate malaria incidences in high transmission areas and secondly, insecticide resistance of the major malaria vectors in Africa is widespread and increasing [3, 4]. Another major concern with these vector control strategies is that these tools are most effective against *Anopheles* vector mosquitoes that feed and rest indoors and have a preference to feed at night. Changes in mosquito host preferences, time of feeding, and an increase in outdoor feeding due to plasticity in mosquito behavioural responses have prompted the need for new and more environmentally friendly robust vector control strategies that supplement current control strategies [2, 5]. The development and incorporation of novel vector control tools based on new scientific knowledge about mosquito behaviour, specifically mosquito semiochemicals (chemical substances that carry messages for purpose of communication), into integrated vector management (IVM) programmes are needed in order to reduce the burden and threat of mosquito-borne diseases [3].

Odour lures for outdoor vector control strategies are currently being used as part of integrated vector control strategies in the fight against malaria. Skin volatiles play an important part in host preferences for specialist feeding behaviour in mosquitoes as these contain host-specific cues [6]. Over 532 skin compounds have been isolated and identified from human skin secretions, however it is unlikely that all the compounds play a role in mosquito-host interactions [7, 8]. Variation in attractiveness between different individuals has been attributed to differences in skin-odour profiles as well as differences in human skin microbial flora [9-11]. Furthermore, the distribution of mosquito bites on human hosts is non-random with the majority of the African mosquito vectors prefering to bite the lower parts of a standing body [12-14]. The variation in human host biting site preference provides another angle to investigate mosquito attraction to humans. The preference of mosquitoes to bite

certain regions on the human host are possible avenues for identifying lead compounds as potential attractants or repellents in push-and-pull vector control strategies.

The importance of skin sampling methods in order to identify skin volatile organic compounds (VOCs) should not be underestimated as VOCs comprise of a broad range of chemicals from various chemical classes with different characteristics. The many inconsistencies reported for detected skin compounds are most likely due to the diverse analytical procedures used, such as variation in sampling protocols, in chromatographic methods, the type of instrumental detector employed, and in data treatment. Sampling procedures range from solvent back extraction from a cotton pad used to swab the sample matrix, dynamic headspace adsorption onto various polymers, solid-phase microextraction (SPME) [7], to recently (2018) sorptive extraction directly from the skin using polydimethylsiloxane (PDMS) loops in the form of bracelets and anklets [15]. Air entrainment, an active sampling technique, was used by Robinson et al. (2018) to determine skin profile differences of healthy and *Plasmodium* infected children [16]. This technique entails the placing of a human body part in a plastic bag and passing air over the skin thus collecting volatile compounds on polymer filters [16]. Mochalski et al. (2018) also employed an active sampling approach which encompassed volunteers to remain seated inside a body chamber, in their underwear, for 2h whilst air from the chamber was analysed [17]. Typically, volunteers have to follow a particular diet and use specific soaps and shampoos before skin sampling [7]. Collection of skin volatiles onto glass beads, worn nylon stockings and T-shirts as sampling methods have also been reported [9, 10, 18-21]. These approaches are most commonly used in combination with gas chromatography coupled to mass spectrometry (GC-MS) [8].

Passive human skin sampling using polydimethylsiloxane (PDMS) samplers in the form of patches or loops has been shown to be reproducible and versatile [15, 22-25]. More importantly sampling with PDMS has been shown to be straightforward and non-invasive. The material is inert, compatible with thermal desorption and degradation products can easily be tracked and identified [26]. Additionally, PDMS is ideal for sampling skin VOCs and semi-VOCs due to the material's ability to concentrate a broad range of analytes from the sampling space through sorptive

extraction. An increase in extraction efficiency of polar compound is also possible, as reported by Ochiai et al. (2016), when modifying a PDMS stir bar with solvent (solvent-assisted stir bar sorptive extraction (SA-SBSE)) [27]. Modification with diethyl ether, methyl isobutylketone, dichloromethane, diisopropyl ether and toluene improved the recoveries for pesticides with a log K_{ow} < 2.5 from an aqueous matrix [27]. These capabilities of PDMS make it ideal for untargeted screening of human skin VOCs and semi-VOCs and for easy non-invasive sampling. Roodt et al. (2018) demonstrated the suitability of using PDMS samplers for determining relative abundances of human skin VOCs and for biomarker discovery [15]. In this present study the difference in chemical profiles between different skin regions is explored with the aim to identify potential lead components for mosquito attractants or repellents. A passive PDMS mini-sampler with thermal desorption thereof directly in the inlet liner of a GC for analysis with comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry (GC×GC-TOFMS) was used for the non-invasive sampling of the human skin surface. The effect of solvent modification of the sampler for improved extraction of polar compounds was investigated to broaden the range of detectable chemical compounds. Furthermore, the feasibility of adding an internal standard by way of solvent modification for improved, meaningful comparison of complex biological data sets was also explored.

3.2. Materials and methods

3.2.1. Reagents and chemical standards

3.2.1.1. Reagents

Methanol (MeOH), *n*-hexane, toluene, acetonitrile (ACN), acetone and isopropanol were all purchased from Merck, South Africa. For linear retention index determination *n*-alkanes C_8-C_{28} were used (Merck, Pretoria, South Africa).

3.2.1.2. Chemical standards

Eucalyptol (1,8-cineole) (Fluka), phenylethyl alcohol (Fluka), heptanal, (*R*)-(+)-β-citronellol, linalool, (-)-carvone, octanal, nonanal, *trans*-2-octenal, *trans*-2-nonenal, *trans*-2-decenal, 3-methyl-2-butenal, 2-octanone, 2-tridecanone, propanoic acid, butanoic acid, indole, terpineol (mixture of isomers), and tetradecanoic acid analytical standards were purchased from Sigma-Aldrich (Pty) Ltd. Kempton Park, South Africa. NLEA FAME mixture, containing hexadecanoic acid, methyl ester, was purchased from Restek (Bellefonte, PA, USA).

3.2.2. Standard solutions

3.2.2.1. Stock solutions

A 100 µg/ml stock solution mixture of the neat liquid standards was prepared by adding 4.9 – 7.2 µl of each standard, as determined by density calculations, in 50 ml of toluene. Individual stock solutions of 100 µg/ml were prepared from solid standards (myristic acid and indole) by dissolving 5 mg powder in 50 mL of toluene. Individual stock solutions of 652 µg/ml eucalyptol and 300 µg/ml FAME mixture were prepared in hexane. All the stock solutions were stored in glass vials and kept at 4 °C.

3.2.2.2. Working solutions

An eucalyptol internal standard (IS) solution of 0.05 µg/ml was prepared by diluting 40 µl of the 652 µg/ml stock solution to a final volume of 500 ml of isopropanol. A working standard solution containing a mixture of the target analytes was prepared at 1 µg/ml in 1 ml of hexane (10 µl of each of the 100 µg/ml stock mixtures (liquid and solid) and 3 µl of the FAME 300 µg/ml stock were diluted to a final volume of 1 ml). All the working solutions were stored in glass vials and kept at 4 °C.

3.2.3. In-house constructed passive PDMS sorptive sampler

A practical, cost-effective disposable mini-sampler was manufactured in-house for passive sorptive extraction of volatile and semi-volatile organic analytes from the human skin surface. The sampler had been previously developed for solvent free extraction of soil [28, 29] and as a passive or dynamic sampler to concentrate pollutants from surface water [30-32]. The samplers (0.060 ± 0.003 g) were fashioned by forming a loop with an 18 cm length of a silicone elastomer medical grade tubing (0.64 mm OD x 0.3 mm ID, Sil-Tec®, Technical Products, Georgia, USA). This length was chosen to allow for effortless use of the sampler as both anklets and bracelets, and to easily fit an inlet liner of a GC. The ends were joined by inserting a 1 cm piece of uncoated silica capillary column (250 µm ID) (SGE Analytical Science, Separation Scientific (Pty) Ltd, Roodepoort, South Africa) [30]. The sorption volume of the loop was 43.87 µl and the internal volume was 13.33 µl. Prior to extraction the PDMS samplers were cleaned and conditioned using the method outlined by Triñanes et al. (2015) for cleaning silicone sampling disks [33]. The PDMS samplers were sonicated three times for 5 minutes each with a MeOH:acetone (1:1, v/v) mixture and then conditioned overnight in a 17.8 cm long glass desorption tube (4 mm ID, 6 mm OD) from Gerstel™ (Chemetrix, Midrand, South Africa) at 250 °C using a Gerstel™ tube conditioner with 100 ml/min hydrogen gas flow. After the overnight conditioning, the loops were sonicated three times for 5 minutes each with ACN and stored dry in a glass vial.

3.2.4. Passive sorptive extraction of human skin volatiles

An IS was added to the PDMS samplers prior to sampling to compensate for any variations, e.g. the size of the sampler, sampling time and instrumental analysis. The sampler loop ends were opened by removing the uncoated capillary coupling and the sampler was then sonicated in 10 ml of the eucalyptol IS in isopropanol solution (0.05 µg/ml). The samplers were removed from the solution with a clean stainless steel tweezer, the surface wiped dry with a lint free tissue and fashioned back into a loop by re-inserting the uncoated capillary coupling. The skin sampling area on a human volunteer was wiped clean with medical grade alcohol cleansing pads (70%

isopropanol, Dischem, South Africa) prior to sampling. Skin volatile samples were collected from a non-smoking Caucasian female, age 31, using the PDMS sorptive sampler. The volunteer's right wrist and ankle were sampled on five consecutive days, using three loops per sampling period of 1 hour (Fig. 1). The samplers were worn as anklets (n=3) and bracelets (n=3) by the volunteer. The sampler was placed in direct contact with the skin, in accordance with Roodt et al. (2018), for ease of sampling, comfort and minimal invasiveness [15]. The sampler was covered with a strip of aluminised Mylar® reflective sheeting (Hydroponic, South Africa), 20 cm x 1.5 cm and 25 cm x 1.5 cm for wrist and ankle skin surface regions, respectively, and kept in place with 3M Micropore medical dressing tape (Dischem, South Africa) (Fig. 1). This present method introduces a barrier to prevent atmospheric contamination of the skin surface and the PDMS sampler during sampling. After sampling the samplers were removed with a clean stainless steel tweezer and individually stored wrapped in aluminium foil at 4 °C for no more than 48 hours before analysis. The sampler was transferred into the inlet liner of a GC for thermal desorption (TD).

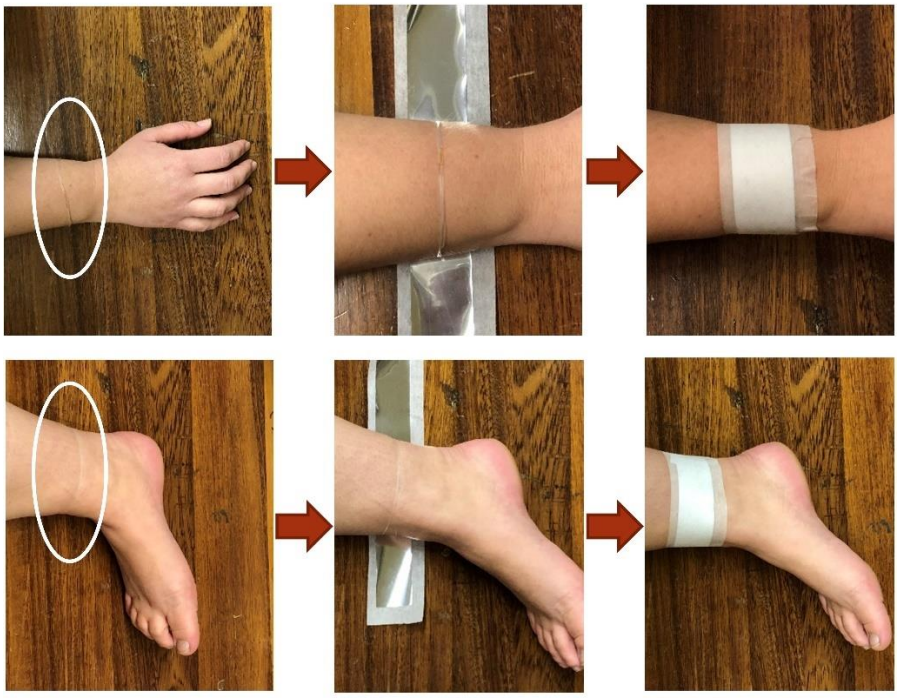

Figure 1. Wrist (top) and ankle (bottom) skin sampling using PDMS samplers worn as bracelets (n=3) and anklets (n=3). The sampler is covered with a strip of aluminised Mylar® reflective sheeting and secured with 3M surgical dressing tape.

The volunteer was asked to continue with her daily routine during the sampling. No effort was made to control the environmental parameters during the sampling. Three method blanks were analysed to account for any laboratory background volatile compounds potentially contaminating the sample during the total procedure before analysis.

3.2.5. Evaluation of the sorptive sampler with and without solvent modification

The influence of modifying the sorptive sampler with solvent when adding the IS solution (0.05 µg/ml isopropanol solution) was evaluated by spiking the sampler, with or without solvent modification, with 19 target analytes (refer to Sections 2.5.1 and 2.5.2.). Isopropanol was specifically selected as a PDMS sampler modifier (IS diluent) in compliance with ethical considerations in terms of low toxicity during human sampling.

3.2.5.1. Spiking procedure: PDMS sorptive sampler without solvent modification

The PDMS sampler without solvent modification was placed on top of a strip of Mylar® reflective sheeting (3 cm x 25 cm) wiped clean with a medical grade alcohol cleansing pad. The mixed working standard solution (1 µg/ml) was spiked onto the Mylar® sheet, next to but not touching the sampler, at three different volumes (1, 5, 10 µl). This resulted in a mass of 1, 5 and 10 ng of each target analyte. Spiking was done in triplicate at the three concentration levels. The Mylar® sheet was folded into a package and secured using 3M dressing tape, whereafter it was placed in a 100 ml Schott glass bottle suspended in a water bath at 31 °C, simulating human skin temperature [34]. After 1 hour the sampler was removed from the Mylar® package with a stainless steel tweezer and stored at 4 °C in aluminium foil until analysis.

3.2.5.2. Spiking procedure: PDMS sorptive sampler with solvent modification

The spiking procedure was repeated for the PDMS sampler modified with isopropanol. The sampler was modified following the same procedure when adding the IS as described in section 2.4. The sampler loop ends were opened by removing the uncoated capillary coupling and sonicated in 10 ml of isopropanol, after which the sampler was removed and fashioned back into a loop by re-inserting the uncoated capillary coupling. The sampler was then placed onto the Mylar® sheet and spiked with the target analytes (5, 10 and 10 ng of each targeted analyte) and extraction commenced following the same procedure as described in section 2.5.1.

The amount of isopropanol added to the PDMS sampler (solvent present as sorbed in the PDMS itself and also in the tubing interior) was determined gravimetrically, in triplicate, as 17 ± 2 mg (22 ± 2 µl). After weighing, the loops were placed in a Schott glass bottle positioned in a water bath at 31°C (to simulate human skin temperature) for an hour, after which the amount of isopropanol remaining was determined gravimetrically to be 11 ± 2 mg (14 ± 3 µl).

3.2.6. Ethical considerations

Written consent was given by the volunteer to participate in the study. No dietary or special hygiene requirements were made. Ethical clearance was provided by the ethics committee of the Faculty of Natural and Agricultural Sciences at the University of Pretoria, South Africa (Reference number EC171109-159).

3.2.7. Comprehensive 2D GC analysis

Separation of compounds was performed on a LECO Pegasus® 4D GC×GC-TOFMS system. The system consists of an Agilent© 7890 GC (LECO Africa (Pty) Ltd., Kempton Park, South Africa) modified to contain a dual stage modulator and

secondary oven. Nitrogen gas cooled with liquid nitrogen was used for the cold jets and synthetic air for the hot jets. The primary column was connected to the secondary column with a presstight column connector (Restek, Bellefonte, PA, USA). ChromaTOF® software (version 4.50.8.0 optimised for Pegasus®, LECO Africa (Pty) Ltd.) was used to operate the instrument and for data capturing and processing. Tentative identification of compounds for untargeted analysis was based on a comparison of sample mass spectra to that of the NIST14 library (version 2.2). Compounds with a spectral match quality of ≥ 80% were reported.

The column set consisted of a Rxi-1 MS 30 m x 0.25 mm ID x 0.25 µm film thickness as the primary column (1D) joined to a Rxi-17Sil MS 1 m x 0.25 mm ID x 0.25 µm film thickness secondary column (2D) (Restek, Bellefonte, PA, USA). The primary oven temperature programme was 40 °C (hold for 1.5 min) at 10 °C/min to 280 °C (hold for 3 min). The GC run time was 28.5 min. The secondary oven was offset by + 5 °C relative to the primary oven. The modulator temperature was offset 15 °C relative to the second oven temperature. The modulation period was 3 s with a hot pulse time of 0.8 s. The carrier gas (helium 5.0, Afrox, South Africa) flow rate was 1.4 ml/min in the constant flow mode. The MS transfer line temperature was set at 280 °C. The ion source temperature was 230 °C, the electron energy was 70 eV in the electron ionisation mode (EI+), the data acquisition rate was 100 spectra/s, the mass acquisition range was 35 – 500 Daltons (Da), and the detector voltage was set at 1533 V. The PDMS sampler was inserted into a splitless-type bottom single taper design (unpacked) glass inlet liner (78.5 mm L × 6.5 mm OD × 4.0 mm ID) (Agilent Chemetrix, Midrand, South Africa) and desorbed in the GC inlet at 250°C with a splitless time of 30 s. The inlet gas flow was shut off prior to manually removing the hot inlet liner from the GC inlet using a pair of tweezers. The PDMS sampler was folded in half before inserting it into the inlet liner, the liner was placed back into the GC inlet, the gas flow restored and the run was started.

Linear retention indices were determined by analysing a mixture of *n*-alkanes (C_8-C_{28}). Experimental linear retention indices were calculated for non-target compounds according to the method of Van den Dool and Kratz (1963) [35]. Compounds within a ±30 RI unit deviation from the literature values were reported.

Peak areas were calculated on the total ion chromatogram (TIC). Limits of detection (LODs) were calculated as those amounts giving a signal to noise ratio (S/N) of 3.

3.2.8. Data processing and statistical analysis

3.2.8.1. Chromatographic peak alignment and comparison

Chromatographic data generated during the initial processing were aligned using ChromaTOF Statistical Compare software (LECO (Pty.)). The mass spectral threshold was set at 800, and the first (1D) and second dimension (2D) retention time deviations were set to 3 and 0.1 s, respectively, for peak alignment. The S/N cut-off was set at 50 for initial peak finding and a secondary cut-off was set at 20 for peaks not aligned during the initial alignment. Principal component analysis (PCA) was done using JMP® Pro 14, a statistical software package from the SAS® Institute Inc. (Cary, North Carolina, USA). PCA was used to visually demonstrate variance between the skin areas sampled, namely ankle and wrist, within the dataset.

3.2.8.2. Peak area normalisation

Peak areas were normalised using the TIC area of the eucalyptol IS when the sampler was modified with solvent containing the IS. During the evaluation of the sampler with and without solvent, the peak areas were normalised using the mass (µg) of the PDMS sampler. Background laboratory volatile compounds from the method blanks were normalised using the IS. The mean (n=3) peak areas of the blanks were then subtracted from the normalised peak areas (normalised using the TIC peak area of the IS) of the human skin volatile compounds.

3.3. Results and discussion

3.3.1. Comparison of the sorptive sampler with and without solvent modification: skin sampling simulation

Nineteen analytical reference standards were selected to investigate the effect of modifying the PDMS sampler with isopropanol as used for the addition of an internal standard. The analytes represent a broad range of compounds (alcohols, aldehydes, carboxylic acids, esters, ketones, nitrogen containing compounds and terpenes) with different polarities (log K_{ow} range: 0.48 – 6.4 (Table 1); with log K_{ow} being the octanol-water partitioning constant). The analytes were selected to simulate the variation in chemical classes and characteristics one would expect when investigating skin VOCs and semi-VOCs during real world human skin surface sampling. Seventeen of the target analytes have previously been detected on human skin and 15 of the target analytes have been reported to elicit a response in mosquitoes (refer to Table 1).

All the target analytes were detected (1, 5, and 10 ng spiking levels) when using either (1) the PDMS sampler without solvent modification or (2) the PDMS sampler with isopropanol modification when simulating the skin surface sampling method (Table 1). For the sampler without solvent modification 71%, 76% and 48% of the compounds for the 1, 5 and 10 ng spike levels, respectively, had a %RSD (n=3) of less than 30%. Whereas for the solvent modified sampler 57%, 72% and 76% of the compounds for the 1, 5 and 10 ng spike levels, respectively, had a %RSD (n=3) of less than 30%. The LODs for the two methods are given in Table 1. LODs without solvent modification ranged from 1 pg for carvone to 241 pg for indole, whilst LODs with solvent modification ranged from 1.2 pg (carvone) to 362 pg (indole). Measurements at ultra-trace levels of the target analytes are realised using either of the methods and thermal desorption directly in the GC inlet liner with GC×GC-TOFMS. The reported LODs obtained with passive absorptive extraction is on average lower than those reported by Veenaas et al. (2020) using active adsorbent extraction of indoor VOCs with GC×GC-TOFMS. On average the LODs were 67 pg for the solvent

modified and 72 pg for the non-solvent methods, whilst Veenaas et al. (2020) reported an average on-tube LOD of 93 pg [36].

No significant observable difference in terms of precision (%RSD) and LODs was found between the PDMS sampler solvent modified or not modified. This could be due to the low volume of isopropanol remaining (14 ± 3 µl) in the sampler after the one-hour sampling period, furthermore, isopropanol could potentially be absorbed by the human skin during sampling. Although an increase in response was demonstrated with increased spiking amounts (in terms of peak areas reported in Table 1) this response showed poor linearity in the range from 1 ng to 5 ng for the majority of the compounds. Compounds at below 5 ng can thus be qualified, but not quantified, when using the GC inlet TD method. However, increasing the concentration from 5 ng to 10 ng using the PDMS sampler with solvent modification all of the target compounds, with the exception of butanoic acid, 3-methyl-2-butanal and octanal, showed linearity in response. For the PDMS sampler without solvent modification 14 of the 19 target compounds demonstrated a linear increase in response. Cryo-focussing is recommended when analysing compounds of molecular weight < 100 Da, and derivatisation is recommended for tetradecanoic acid, to improve linearity or repeatability of these compounds. Manual handling and insertion of the loop using a stainless-steel tweezer into the GC inlet liner may explain disparities in the %RSDs reported for low molecular weight compounds (Table 1). Of interest is the increase in response for linalool, (*E*)-2-nonenal, nonanal and (*E*)-2-decenal at 10 ng spike for the solvent modified sampler, whilst the without solvent modification method appeared to reach a plateau prior to 10 ng. The reason for this is not clear. This could be due to an increase in the analyte capacity of the sampler with solvent addition (the PDMS sorbent volume in addition to the solvent volume compared to only PDMS sorbent) when doing solvent modifications. The PDMS sampler (without solvent modification) appears to reach its analyte capacity, resulting in a reduced sensitivity, prior to 10 ng; a level higher than what is required for the detection of skin VOCs and semi-VOCs.

The internal standard reponse showed excellent precision (%RSD) during the five day sampling period. %RSD was determined using the TIC peak area of the eucalyptol internal standard. The within run precision (n=3) was 6.6% (287515419 ± 19143736) and the between run precision (n=29) was 9.2% (299742542 ± 27687442).

Application of the Dixon Q-test identified no peak area values as outliers at a 95% confidence level (Q_{crit} = 3.65; Q_{stat} = 0.522 for the lowest TIC peak area value and Q_{stat} = 0.478 for the highest TIC peak area value; $Q_{stat} < Q_{crit}$ and therefore no peak areas were rejected as outliers).

Table 1. Method comparison of the PDMS sorptive sampler modified with isopropanol or without isopropanol. Mean, standard deviation and %RSD (n=3) of the mass normalised TIC peak areas at 1 ng, 5 ng and 10 ng spiked on sampler with the target analytical standards and using a skin sampling simulation with GC inlet TD and GC×GCTOFMS. Log K_{ow} and LODs (pg) are given for the target analytes.

Analyte	Log K_{ow}	1 ng		5 ng		10 ng		LODs (pg)
		$\bar{x} \pm \sigma_{n=3}$	%RSD	$\bar{x} \pm \sigma_{n=3}$	%RSD	$\bar{x} \pm \sigma_{n=3}$	%RSD	
PDMS sampler without solvent modification								
Propanoic acid[a, b]	0.48	4.1[c] ± 1.3	30	27 ± 9.6	36	33 ± 26	77	1.7
Butanoic acid[a, b]	0.92	0.89 ± 0.28	31	5.6 ± 1.5	27	6.6 ± 2.4	36	-[d]
2-Butenal, 3-methyl[a]	1.00	0.068 ± 0.070	103	0.31 ± 0.11	37	0.75 ± 0.19	25	91
Phenylethyl alcohol[a,b]	1.49	31 ± 5.6	18	93 ± 18	19	120 ± 50	42	1.3
Indole[a, b]	2.07	5.7 ± 0.68	12	10 ± 2.0	20	30 ± 2.3	8	241
Heptanal[a]	2.10	13 ± 1.7	13	17 ± 0.47	3	21 ± 0.73	3	-[e]
Terpineol[a, b]	2.17	29 ± 7.6	26	34 ± 6.7	20	68 ± 19	27	1.9
Octanal[a, b]	2.54	21 ± 7.3	34	28 ± 5.4	19	57 ± 22	39	42
(*E*)-2-Octenal[a]	2.54	11 ± 2.7	24	29 ± 4.7	16	45 ± 15	33	28
Carvone	2.55	14 ± 4.4	32	38 ± 1.3	3	81 ± 46	57	1
2-Octanone[a, b]	2.59	25 ± 7.0	28	64 ± 6.6	10	113 ± 42	37	1.8
Linalool[a, b]	2.65	18 ± 2.9	16	35 ± 4.7	13	38 ± 2.2	6	-[e]
(*R*)-(+)-β-citronellol[a, b]	2.75	5.2 ± 1.2	23	11 ± 0.60	5	23 ± 6.1	26	6.5
(*E*)-2-Nonenal[a, b]	2.98	4.0 ± 0.51	13	8.6 ± 0.87	10	11 ± 0.37	3	6.1
Nonanal[a, b]	2.99	16 ± 4.8	30	17 ± 2.0	12	16 ± 0.32	2	-[e]
(*E*)-2-Decenal[b]	3.43	6.6 ± 1.8	27	11 ± 0.87	8	14 ± 2.2	15	28
2-Tridecanone[a, b]	4.81	16 ± 3.6	23	38 ± 4.7	12	112 ± 54	48	2.0
Tetradecanoic acid[a, b]	5.37	6.8 ± 2.9	42	9.1 ± 4.0	44	5.5 ± 2.7	49	-[e]
Hexadecanoic acid, methyl ester[a, b]	6.40	3.3 ± 0.13	4	4.6 ± 0.16	4	7.3 ±0.58	8	9.5
PDMS sampler with solvent modification								
Propanoic acid[a, b]	0.48	2.9 ± 0.7	25	6.0 ± 1.3	22	12 ± 2.1	17	21
Butanoic acid[a, b]	0.92	2.2 ± 2.4	109	1.9 ± 2.6	134	1.3 ± 1.0	75	-[d]
2-Butenal, 3-methyl[a]	1.00	2.1 ± 0.42	20	0.76 ± 0.16	21	0.96 ± 0.030	3	-[d]
Phenylethyl alcohol[a,b]	1.49	28 ± 4.7	17	52 ± 13	25	152 ± 45	29	3.3
Indole[a, b]	2.07	4.6 ± 1.8	38	21 ± 6.9	32	36 ± 6.2	18	362
Heptanal[a]	2.10	7.8 ± 3.0	38	11 ± 1.9	18	19 ± 0.92	5	13
Terpineol[a, b]	2.17	45 ± 0.91	2	37 ± 8.0	21	62 ± 13	21	2.6
Octanal[a, b]	2.54	24 ± 21	88	18 ± 14	78	18 ± 9.2	51	-
(*E*)-2-Octenal[a]	2.54	21 ± 10	51	35 ± 2.4	7	67 ± 14	21	48
Carvone	2.55	13 ± 3.2	25	36 ± 7.2	20	93 ± 33	36	1.2

Analyte	Log K_{ow}	1 ng		5 ng		10 ng		LODs (pg)
		$\bar{x} \pm \sigma_{n=3}$	%RSD	$\bar{x} \pm \sigma_{n=3}$	%RSD	$\bar{x} \pm \sigma_{n=3}$	%RSD	
2-Octanone[a, b]	2.59	17 ± 5.5	33	40 ± 6.0	15	78 ± 17	22	3.6
Linalool[a, b]	2.65	21 ± 4.9	24	31 ± 5.1	16	67 ± 11	17	1.9
(*R*)-(+)-β-citronellol[a, b]	2.75	5.2 ± 0.83	16	8.8 ± 0.87	16	20 ± 4.4	22	9.8
(*E*)-2-Nonenal[a, b]	2.98	2.6 ± 0.27	10	6.3 ± 1.2	19	18 ± 1.9	10	12
Nonanal[a, b]	2.99	15 ± 0.51	3	16 ± 3.3	20	26 ± 1.2	5	18
(*E*)-2-Decenal[b]	3.43	5.0 ± 0.41	8	12 ± 1.5	12	28 ± 0.18	1	18
2-Tridecanone[a, b]	4.81	16 ± 3.2	20	38 ± 9.0	24	78 ± 17	22	1.6
Tetradecanoic acid[a, b]	5.37	7.4 ± 2.9	40	4.0 ± 1.3	34	6.7 ± 2.5	37	15
Hexadecanoic acid, methyl ester[a, b]	6.40	2.6 ± 0.36	15	3.3 ± 0.31	10	5.3 ± 0.97	19	8.8

LODs are expressed as concentrations giving a S/N of 3 as calculated from the spiked samplers at 5 ng

a) Previously reported on human skin [8, 15, 37-39]
b) Response reported in mosquitoes [5, 11, 37, 40-56]
c) Mean peak area (TIC) normalised using mass (µg) of PDMS sampler
d) Cryo-focussing is recommended
e) Non-linear response

3.3.2. Untargeted analysis

An untargeted analysis of the human skin surface, from the ankle and wrist area, of a volunteer sampled for one hour per day over a five-day period using a sorptive PDMS sampler and GC inlet TD followed by GC×GC-TOFMS yielded an exhaustive list of VOCs and semi-VOCs. Over 1 800 compounds from a broad range of chemical classes were detected using the non-invasive PDMS sampler together with the superior resolving power and sensitivity of GC×GC-TOFMS. Compounds detected included aldehydes, alkanes, alkenes, alcohols, ethers, carboxylic acids, esters, and nitrogen containing compounds as well as exogenous skin compounds such as terpenes, polyaromatic hydrocarbons (PAHs), parabens, and phthalates. The compound list was filtered using an ≥80% mass spectra match quality criterion and by removal of background contaminants (including all siloxanes interpreted as PDMS artefacts) yielding a final list of 545 tentatively identified compounds or features. These compounds represent a range of compounds amenable to PDMS extraction. The list of 545 compounds is given in the Supporting Information Table S1. Exogenous compounds were retained to provide a comprehensive skin chemical profile, moreover, the influence of these compounds on mosquito behavioural

responses has to be considered. For example, the plant volatile linalool was detected on the skin and is reported to elicit a strong antennal response in *Cx. pipiens* and *Ae. aegypti* mosquito species [57]. Verhulst et al. (2016) stated that when volunteers stopped using skincare products prior to skin sampling no difference in attraction of *An. coluzzi* to different body parts was detected, concluding that skincare products may affect an individual's attractiveness to mosquitoes [47].

3.3.2.1. Comparison of ankle and wrist skin chemical profiles

The chemical profiles between the two skin surface regions, ankle and wrist, differed significantly. Representative contour plots (TIC) (GC×GC-TOFMS) for the two skin regions are provided in the Supplementary Information Fig. S1. Principal component analysis was conducted using the normalised peak area of the 545 compounds to visualise variances between the two skin regions sampled (Fig. 2). The 545 compounds were consequently analysed using LECO ChromaTOF Statistical Compare software to identify the features contributing to the difference in the skin chemical profiles of the ankle and wrist skin surface area. Statistical Compare uses Fisher ratios as a simple method to identify significant differences between the two classes investigated. The Fisher ratio is the ratio of between-class variance, also called class-to-class variance, to within-class variance. The analyses yielded 86 compounds that contributed to the difference between the two skin regions. These compounds, mean peak areas were all normalised using the IS for improved reliable comparisons, are given in Table 2. The compounds are from a broad range of chemical classes and were tentatively identified or putatively annotated (this type of identification refers to a level two identification when using the metabolomics standards initiative on metabolite identification) based on mass spectral library matches and were further confirmed by corresponding first dimension linear retention indices (LRIs). On average the agreement between experimental and database LRIs was ±2 RI units (standard deviation ±8 RI units). These results are in line with results obtained from a non-targeted indoor VOCs study using GC×GC coupled to a high-resolution mass spectrometer

[36]. The authors reported an average agreement of within eight RI units and a standard deviation of ±23 RI units [36]. Compounds that were closely associated with the wrist included 6-methyl-1-heptanol, 3-(4-isopropylphenyl)-2-methylpropionaldehyde, 2-phenoxyethyl isobutyrate, and 2,4,6-trimethyl-pyridine. These compounds were detected on four of the five days on the wrist skin surface area, whilst they were not detected on the ankle skin surface area. Conversely, compounds detected exclusively on the ankle region included 2-butoxyethanol phosphate, 2-heptanone, and *p*-menthan-8-ol. 2-Butoxyethanol phosphate and *p*-menthan-8-ol were detected on four of the five days and 2-heptanone was detected on three of the five days on the ankle skin surface region; all three compounds were never detected on the wrist skin surface area. Results are noteworthy and may provide potential lead compounds for repellents or attractants. To the best of the authors' knowledge 46 of the 86 compounds have not previously been reported on the human skin surface (Table 2).

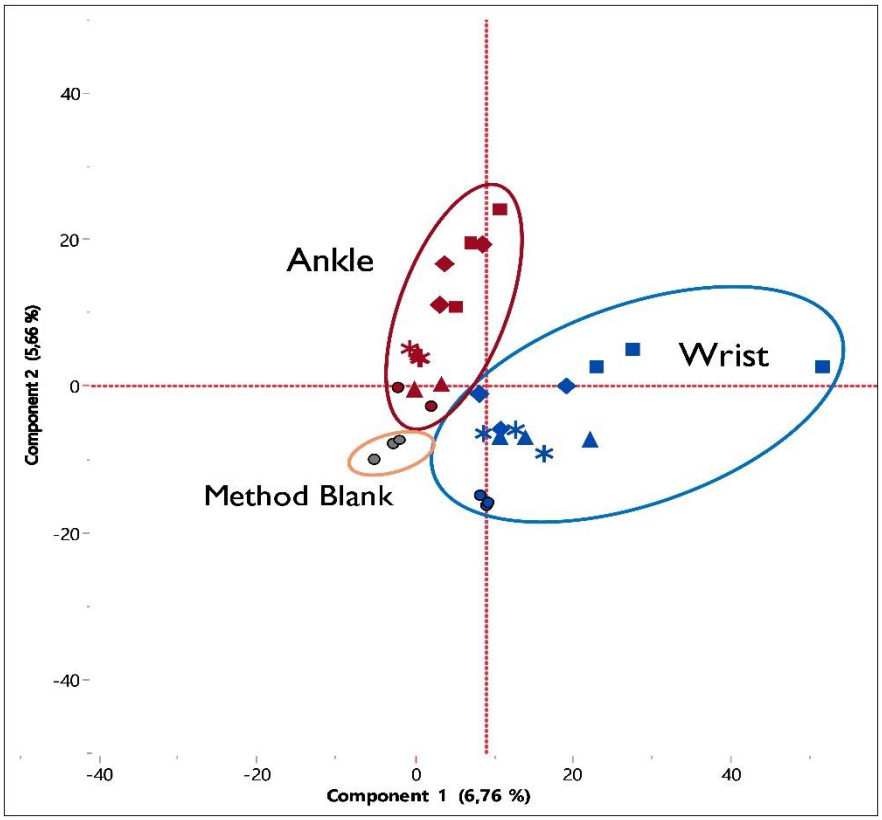

Figure 2. Principal component analysis on 545 compounds was used to graphically demonstrate the variance in the chemical profiles of the human skin regions sampled, wrist (blue) and ankle (red). Sampling was performed for one hour using three replicate PDMS samplers (n=3) per day over five days and analysed with a GC×GC-TOFMS. Score data points are represented by circles for day 1; stars for day 2; triangles for day 3, squares for day 4; diamonds for day 5. Single event method blanks (n=3), grey circles, were done to account for any background laboratory volatile compounds.

Table 2. Compounds tentatively identified during an untargeted analysis of the human skin surface originating from the ankle and wrist area using an in-house developed PDMS sampler with inlet TD-GC×GC-TOFMS. The compounds listed are limited to those that were classified by LECO ChromaTOF Statistical Compare software as contributing to the difference, using Fisher ratios, between the ankle and wrist skin surface chemical profile.

								Wrist (m=15)[a]					Ankles (m=14)[a, b]			
#	Compound	CAS Number	1D RT[c] (s)	2D RT[d] (s)	1D RI_{exp}	1D RI_{Lit} NIST14	Previously reported on skin	Count (n=5)[e]	Mean[f]	Median	Range Min	Range Max	Count (n=5)[e]	Mean	Median	Range Min	Range Max
Alkanes																	
1	Nonane	111-84-2	342	0.63	900	900	[8, 37, 39]	2	0.0790	0.0790	0.0457	0.1122	4	0.0839	0.0883	0.0223	0.1367
2	Pentadecane, 2-methyl-	1560-93-6	912	0.70	1571	1565	n/a[g]	1	0.1822	0.1822	0.1822	0.1822	0	n.d.[h]	n.d.	n.d.	n.d.
3	Docosane	629-97-0	1295	0.75	2200	2203	[8]	2	0.9222	0.9222	0.2186	1.6258	1	1.0983	1.0983	1.0983	1.0983
Alkenes																	
4	1,3-Octadiene	1002-33-1	267	0.68	822	820	n/a	0	n.d.	n.d.	n.d.	n.d.	1	0.0845	0.0845	0.0845	0.0845
5	3-Tetradecene, (*Z*)-	41446-67-7	783	0.73	1393	1395	n/a	1	0.2895	0.2895	0.2895	0.2895	1	0.1275	0.1275	0.1275	0.1275
6	8-Heptadecene	2579-04-6	1014	0.75	1723	1719	n/a	1	0.0825	0.0825	0.0825	0.0825	0	n.d.	n.d.	n.d.	n.d.
Alcohols																	
7	Phenol, 2-methyl-	95-48-7	496	1.13	1039	1062	[15]	1	0.0733	0.0733	0.0733	0.0733	0	n.d.	n.d.	0	0
8	Ethanol, 2-butoxy-	111-76-2	327	1.05	884	890	n/a	3	1.7043	1.4961	0.1223	3.4944	2	1.7530	1.7530	0.1560	3.3500
9	1-Heptanol, 6-methyl-	1653-40-3	420	0.84	995	981	n/a	4	0.8499	0.8145	0.0072	1.7633	0	n.d.	n.d.	n.d.	n.d.
10	Phenol, 2-methyl-5-(1-methylethyl)-	499-75-2	684	1.10	1273	1279	n/a	3	0.0296	0.0133	0.0124	0.0632	0	n.d.	n.d.	n.d.	n.d.
11	Cyclohexanol, 1-methyl-4-(1-methylethyl)-	21129-27-1	588	0.94	1161	1156	n/a	2	0.0808	0.0808	0.0242	0.1374	0	n.d.	n.d.	n.d.	n.d.
12	Patchouli alcohol	5986-55-0	969	1.18	1655	1656	n/a	1	0.0449	0.0449	0.0449	0.0449	0	n.d.	n.d.	n.d.	n.d.
13	Hexadecen-1-ol, trans-9-	64437-47-4	1107	0.87	1862	1869	n/a	2	0.7636	0.7636	0.0219	1.5053	5	0.4614	0.2399	0.0097	1.0792
14	1-Hexadecanol	36653-82-4	1107	0.89	1880	1871	[8]	3	1.1704	1.1761	0.8843	1.4506	1	0.8189	0.8189	0.8189	0.8189

Benzyl and phenyl hydrocarbons																
15	*o*-Xylene	95-47-6	309	0.91	866	881	n/a	1	0.0103	0.0103	0.0103	0.0103	0	n.d.	n.d.	n.d.	n.d.
16	Benzene, 1-ethyl-3-methyl-	620-14-4	390	0.87	950	950	n/a	2	0.7116	0.7116	0.1657	1.2575	2	0.0431	0.0431	0.0114	0.0747
17	Benzene, 1-methyl-3-propyl-	1074-43-7	477	0.87	1042	1042	n/a	3	0.0425	0.0501	0.0031	0.0742	2	0.3399	0.3399	0.1602	0.5196
18	*o*-Cymene	527-84-4	502	0.91	1042	1069	[58]	1	0.0329	0.0329	0.0329	0.0329	1	0.1745	0.1745	0.1745	0.1745
19	Biphenyl	92-52-4	753	1.33	1356	1366	n/a	1	0.0011	0.0011	0.0011	0.0011	4	0.0048	0.0047	0.0001	0.0095
20	Benzene, (1-ethylnonyl)-	4536-87-2	972	0.88	1659	1656	[8]	1	0.0718	0.0718	0.0718	0.0718	2	0.0716	0.0716	0.0124	0.1309
21	Benzene, (1-pentylhexyl)-	4537-14-8	951	0.86	1627	1624	n/a	1	0.1377	0.1377	0.1377	0.1377	2	0.0956	0.0956	0.0175	0.1737
22	Benzene, (1-pentyloctyl)-	4534-49-0	1077	0.86	1820	1817	[8]	2	0.156	0.156	0.0258	0.2862	2	0.2106	0.2106	0.1315	0.2897
Poly aromatic hydrocarbons (PAHs)																	
23	Naphthalene, 1-methyl-	90-12-0	687	1.27	1276	1290	n/a	1	0.0176	0.0176	0.0176	0.0176	1	0.0024	0.0024	0.0024	0.0024
24	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	2809-64-5	687	1.16	1276	1280	n/a	0	n.d.	n.d.	n.d.	n.d.	1	0.0067	0.0067	0.0067	0.0067
25	Acenaphthene	83-32-9	831	1.47	1458	1463	n/a	2	0.0002	0.0002	0.0001	0.0003	1	0.0006	0.0006	0.0006	0.0006
26	Naphthalene, 2-ethyl-	939-27-5	769	1.30	1390	1376	n/a	0	n.d.	n.d.	n.d.	n.d.	2	0.0011	0.0011	0.0008	0.0015
27	9H-Xanthene	92-83-1	942	1.40	1614	1628	n/a	1	0.0002	0.0002	0.0002	0.0002	0	n.d.	n.d.	n.d.	n.d.
Aldehydes																	
28	2-Pentenal, 2-methyl-	623-36-9	258	0.89	813	810	n/a	1	0.0206	0.0206	0.0206	0.0206	0	n.d.	n.d.	n.d.	n.d.
29	Benzaldehyde, 4-methyl-	104-87-0	489	1.30	1055	1069	n/a	5	0.0244	0.0085	0.0033	0.0821	2	0.0075	0.0075	0.0034	0.0115
30	Benzeneacetaldehyde	122-78-1	450	1.36	1013	1011	[15]	2	0.0287	0.0287	0.0144	0.043	4	0.0586	0.0693	0.0044	0.0913
31	Octanal	124-13-0	423	0.90	984	982	[8, 15, 37, 39]	4	0.9506	0.9288	0.7263	1.2186	5	1.1213	1.285	0.4831	1.7305
32	Cinnamaldehyde, (*E*)-	14371-10-9	654	1.51	1236	1237	n/a	1	0.0006	0.0006	0.0006	0.0006	1	0.0018	0.0018	0.0018	0.0018
33	2,4-Nonadienal, (*E,E*)-	5910-87-2	615	1.07	1190	1188	n/a	2	0.0010	0.0010	0.0008	0.0013	0	n.d.	n.d.	n.d.	n.d.
34	2-Nonenal, (*E*)-	18829-56-6	567	0.98	1139	1135	[8, 39]	5	0.0559	0.0522	0.0189	0.0873	5	0.0921	0.0841	0.0212	0.2029
35	Piperonal	120-57-0	705	1.65	1298	1299	n/a	3	0.0040	0.0028	0.0014	0.0080	1	0.0013	0.0013	0.0013	0.0013
36	2-Undecenal	2463-77-6	744	0.95	1345	1344	[15]	2	0.0384	0.0384	0.0176	0.0592	0	n.d.	n.d.	n.d.	n.d.
37	Dodecanal	112-54-9	780	0.89	1389	1389	[8]	3	0.0657	0.0363	0.0342	0.1265	1	0.0427	0.0427	0.0427	0.0427
38	3-(4-Isopropylphenyl)-2-methylpropionaldehyde	103-95-7	813	1.19	1433	1424	n/a	4	0.0112	0.0102	0.0051	0.0194	0	n.d.	n.d.	n.d.	n.d.

Ethers																
39	2-Furancarboxaldehyde, 5-methyl-	620-02-0	378	1.30	938	933	[15]	2	0.0192	0.0192	0.0052	0.0332	0	n.d.	n.d.	n.d.	n.d.
40	Vanillin	121-33-5	756	1.66	1360	1360	n/a	5	0.0020	0.0017	0.0006	0.0046	3	0.0024	0.0025	0.0021	0.0028
41	Safrole	94-59-7	681	1.22	1269	1269	n/a	4	0.0295	0.0256	0.0173	0.0493	1	0.0029	0.0029	0.0029	0.0029
Ketones																	
42	Cyclohexanone	108-94-1	309	1.16	866	871	n/a	0	n.d.	n.d.	n.d.	n.d.	1	0.0447	0.0447	0.0447	0.0447
43	2-Heptanone	110-43-0	312	0.87	869	869	[15, 37]	0	n.d.	n.d.	n.d.	n.d.	3	0.1738	0.1992	0.0195	0.3028
44	Levoglucosenone	37112-31-5	501	1.79	1068	1070	n/a	2	0.0077	0.0077	0.0010	0.0144	0	n.d.	n.d.	n.d.	n.d.
45	2-Octanone	111-13-7	414	0.88	975	971	[15]	5	1.1737	0.8767	0.033	3.0408	3	0.6431	0.8546	0.1978	0.8770
46	2-Butanone, 4-(4-hydroxyphenyl)-	5471-51-2	873	1.61	1517	1498	n/a	1	0.0276	0.0276	0.0276	0.0276	0	n.d.	n.d.	n.d.	n.d.
47	2-Undecanone	112-12-9	690	0.89	1280	1273	[8, 15]	3	0.0518	0.046	0.0341	0.0752	2	0.0301	0.0301	0.0133	0.0470
48	3-Dodecanone	1534-27-6	768	0.88	1375	1369	n/a	3	0.0497	0.0374	0.0094	0.1024	0	n.d.	n.d.	n.d.	n.d.
49	3,5,9-Undecatrien-2-one, 6,10-dimethyl-	141-10-6	906	1.08	1563	1553	n/a	1	0.0021	0.0021	0.0021	0.0021	0	n.d.	n.d.	n.d.	n.d.
50	2-Tridecanone	593-08-8	849	0.89	1483	1477	[8, 15, 39]	5	0.0784	0.0696	0.0288	0.1313	5	0.0266	0.0209	0.0089	0.0628
51	3-Tridecanone	1534-26-5	843	0.88	1475	1470	n/a	2	0.0550	0.0550	0.0497	0.0604	0	n.d.	n.d.	n.d.	n.d.
Carboxylic acids																	
52	Hexanoic acid, 2-ethyl-	149-57-5	553	0.85	1128	1123	[8, 15]	3	0.3665	0.4250	0.1778	0.4967	5	0.1889	0.1091	0.0055	0.4458
53	*n*-Decanoic acid	334-48-5	753	0.94	1372	1357	[8, 15]	4	0.1817	0.1573	0.0107	0.4016	2	0.5093	0.5093	0.1988	0.8198
54	Benzoic acid, *p*-tert-butyl-	98-73-7	852	1.09	1488	1479	[8, 15]	2	0.0052	0.0052	0.0051	0.0053	1	0.0010	0.0010	0.0010	0.0010
55	Nonadecanoic acid	646-30-0	1317	0.92	2248	2236	[8, 15]	3	0.0741	0.0351	0.0111	0.1762	1	0.0776	0.0776	0.0776	0.0776
Esters																	
56	Butyrolactone	96-48-0	309	1.88	866	867	[15, 37]	1	0.0004	0.0004	0.0004	0.0004	1	0.0114	0.0114	0.0114	0.0114
57	Propylene carbonate	108-32-7	372	2.07	931	931	[8, 15]	0	n.d.	n.d.	n.d.	n.d.	2	0.0098	0.0098	0.0074	0.0123
58	Dehydromevalonic lactone	2381-87-5	546	1.94	1116	1114	[8, 15]	0	n.d.	n.d.	n.d.	n.d.	1	0.0012	0.0012	0.0012	0.0012
59	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	543	1.52	1113	1108	[8]	3	0.0042	0.0044	0.0010	0.0072	1	0.0028	0.0028	0.0028	0.0028
60	1,2,3-Propanetriol, 1-acetate	106-61-6	522	1.28	1090	1091	n/a	1	0.0028	0.0028	0.0028	0.0028	0	n.d.	n.d.	n.d.	n.d.
61	Benzoic acid, methyl ester	93-58-3	507	1.21	1074	1072	n/a	1	0.0006	0.0006	0.0006	0.0006	2	0.0062	0.0062	0.0015	0.0110
62	2-Butoxyethyl acetate	112-07-2	504	0.97	1071	1066	n/a	1	0.0161	0.0161	0.0161	0.0161	2	0.1709	0.1709	0.1599	0.1818

63	Styrallyl acetate	93-92-5	594	1.17	1168	1166	n/a	3	0.0196	0.0162	0.0064	0.0361	0	n.d.	n.d.	n.d.	n.d.
64	Benzeneethanol, à,à-dimethyl-, acetate	151-05-3	708	1.08	1302	1298	n/a	1	0.0034	0.0034	0.0034	0.0034	0	n.d.	n.d.	n.d.	n.d.
65	Bornyl acetate	76-49-3	687	0.98	1276	1270	n/a	3	0.0165	0.0192	0.0084	0.0219	0	n.d.	n.d.	n.d.	n.d.
66	Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester, *cis*-	19464-95-0	861	1.29	1500	1484	n/a	1	0.0116	0.0116	0.0116	0.0116	0	n.d.	n.d.	n.d.	n.d.
67	2-Phenoxyethyl isobutyrate	103-60-6	852	1.22	1488	1488	n/a	4	0.0229	0.0132	0.0083	0.0567	0	n.d.	n.d.	n.d.	n.d.
68	Pentanoic acid, 2,2,4-trimethyl-3-hydroxy-, isobutyl ester	244074-78-0	741	1.03	1342	1331	n/a	2	0.1773	0.1773	0.0493	0.3054	2	0.0343	0.0343	0.0332	0.0354
69	Butanoic acid, 1,1-dimethyl-2-phenylethyl ester	10094-34-5	843	1.04	1475	1476	n/a	1	0.0148	0.0148	0.0148	0.0148	0	n.d.	n.d.	n.d.	n.d.
70	Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	24851-98-7	966	1.22	1650	1657	[8]	1	0.0332	0.0332	0.0332	0.0332	0	n.d.	n.d.	n.d.	n.d.
71	Phenylethyl salicylate	87-22-9	1140	1.50	1925	1934	n/a	1	0.0030	0.0030	0.0030	0.0030	0	n.d.	n.d.	n.d.	n.d.
72	Hexadecanoic acid, methyl ester	112-39-0	1134	0.87	1915	1909	[8, 38]	4	0.3005	0.2655	0.0977	0.5733	5	0.1687	0.1468	0.1111	0.2481
73	Benzyl butyl phthalate	85-68-7	1341	1.69	2297	2290	n/a	3	0.0025	0.0023	0.0002	0.0051	4	0.0165	0.0160	0.0037	0.0301
Terpenes																	
74	Limonene	138-86-3	462	0.79	1026	1017	[37, 38, 58]	2	0.0371	0.0227	0.0122	0.0764	1	0.4089	0.4089	0.4089	0.4089
75	Linalool	78-70-6	522	0.88	1090	1086	[8, 15]	4	0.5598	0.5250	0.5598	0.6754	2	0.5508	0.5508	0.5317	0.5700
76	Terpineol	8000-41-7	603	1.01	1175	1177	[58]	5	0.1116	0.1052	0.0780	0.1570	5	0.3498	0.3106	0.1768	0.5489
77	Citronellol	106-22-9	636	0.93	1215	1211	[8]	5	0.0635	0.0699	0.0158	0.1007	5	0.0535	0.0562	0.0212	0.0786
78	*p*-Menthan-8-ol	498-81-7	564	0.92	1162	1135	n/a	0	n.d.	n.d.	n.d.	n.d.	4	0.0816	0.0524	0.0047	0.2170
Halogen containing volatiles																	
79	Benzene, 1,3-dichloro-	541-73-1	429	1.14	991	989	n/a	2	0.0012	0.0012	0.0007	0.0017	1	0.2157	0.2157	0.2157	0.2157
Nitrogen containing volatiles																	
80	Ethanone, 1-(1H-pyrrol-2-yl)-	1072-83-9	471	1.41	1035	1030	n/a	0	n.d.	n.d.	n.d.	n.d.	2	0.0426	0.0426	0.0075	0.0777
81	Indole	120-72-9	675	1.64	1262	1273	[8, 15]	5	0.0053	0.0044	0.0033	0.0080	5	0.0080	0.0088	0.0044	0.0110
82	Pyridine, 2,4,6-trimethyl-	108-75-8	420	1.05	981	977	n/a	4	0.1903	0.1682	0.1638	0.2611	0	n.d.	n.d.	n.d.	n.d.
83	o-Cyanobenzoic acid	3839-22-3	807	1.86	1425	1428	n/a	1	0.0010	0.0010	0.0010	0.0010	1	0.0018	0.0018	0.0018	0.0018
84	1,7-Dimethylxanthine	611-59-6	1101	2.13	1860	1851	n/a	0	n.d.	n.d.	n.d.	n.d.	2	0.0082	0.0082	0.0026	0.0139

Phosphor containing volatiles																
85	Ethanol, 2-butoxy-, phosphate (3:1)	78-51-3	1377	1.20	2370	2363	n/a	0	n.d.	n.d.	n.d.	n.d.	4	0.0043	0.0041	0.0007	0.0084
Sulphur containing volatiles																
86	2-Undecanethiol, 2-methyl-	10059-13-9	816	0.71	1438	1433	n/a	3	0.1137	0.0554	0.0494	0.2363	1	0.0777	0.0777	0.0777	0.0777

a) Number of measurements taken
b) Ankle observations m=14 (not 15) due to power outages
c) First dimension retention time
d) Second dimension retention time
e) Number of days (n=5) compound was detected
f) Peak areas were normalised using the TIC of the eucalyptol IS
g) n/a = not available
h) Not detected

3.3.2.2. Detection of mosquito semiochemicals

African malaria vector mosquitoes show a biting preference towards the lower parts of their human hosts with the selection of biting sites mediated by host odour cues [13, 14, 59, 60]. A list of semiochemicals (43) previously reported to elicit a response in mosquitoes (refer to Wooding et al. (2020) for a comprehensive list of mosquito semiochemicals [56]) and detected during this study is given in in the Supporting Information Table S2. Tetradecanoic acid (Fig. 3) was more abundant on the wrist area than the ankle area. This agrees with findings from Verhulst et al. (2016) and Roodt et al. (2018) [15, 47]. Of interest is that tetradecanoic acid is used in a three-component odour blend known to be attractive to *An. gambiae* mosquitoes [42, 44] and it is associated with highly mosquito attractive individuals [41]. The higher presence of tetradecanoic acid on the wrist skin area, an area that is seen as unattractive for mosquitoes, is therefore not as was anticipated for this mosquito attractive compound. This leads to the conclusion that single compounds on their own are not the only criterion involved in attraction. It is important to note that some studies have shown the preference of African vector mosquitoes to bite their human host closer to the ground level, i.e. when lying down biting sites are often random as compared to sitting when mainly the legs and feet are bitten. This led to the conclusion that convection currents, and as well as odour cues, play a role during the final biting site selection [13, 14, 59].

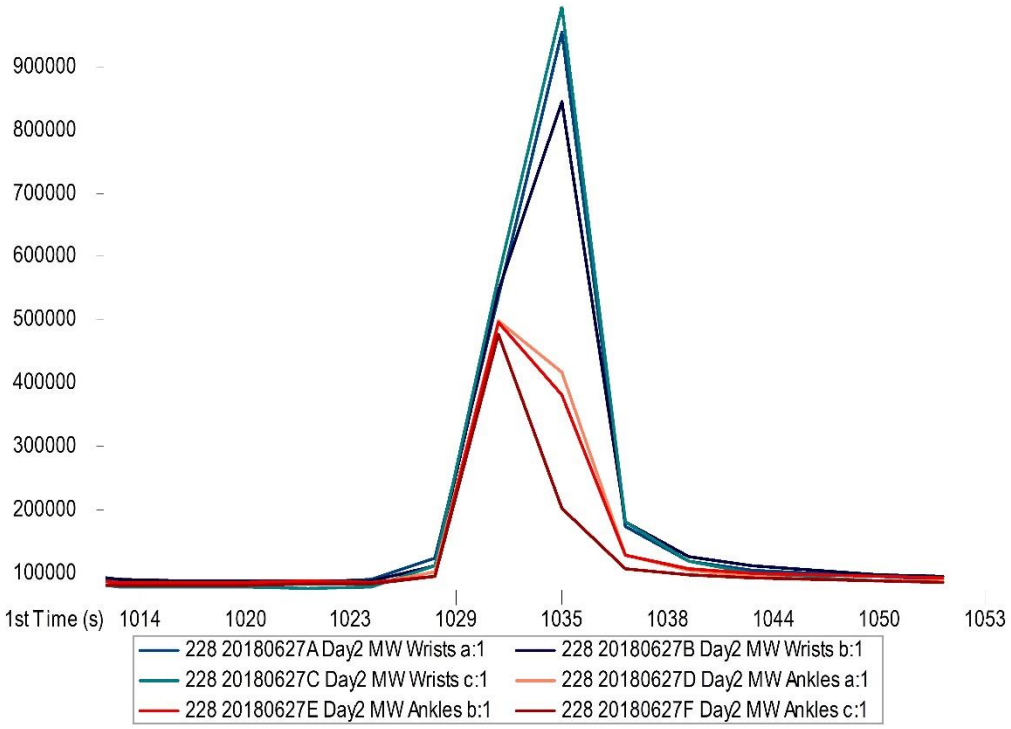

Figure 3. First dimension reconstructed ion chromatogram (RIC) (228 *m/z*) (GC×GC-TOFMS) of tetradecanoic acid detected on human skin sampled on Day 2. The top three traces show the detection of the analyte on the wrist (n=3) and the bottom three traces show the detection of the analyte on the ankle (n=3) of a volunteer; demonstrating the difference in peak area abundance obtained of the mosquito semiochemical, tetradecanoic acid, between the two skin surface areas sampled.

The type of response elicited in mosquitoes by semiochemicals and the synergistic effect is of interest when formulating new attractants and repellents. Nonanoic acid was detected on the wrist on all five days sampled and only detected on the ankle on two of the five days sampled. The abundance on the wrist was also higher than on the ankle. This is of interest as carboxylic acids are often used synergistically as attractants in mosquito odour lures highlighting the importance of synergism when developing these lures [44]. An antennal response was detected in female *An. gambiae* mosquitoes when exposed to 2-phenoxy-ethanol [50]. Whether the mosquito response was attractive or repellent was not determined [50]. This compound was detected on all five days on the wrist area and only once on the ankle area. 2-Octanone, which

was present in higher abundance on the wrist area, has been shown to reduce the attractiveness of a mosquito odour lure [61]. Palmitoleic acid was detected in a significantly higher abundance on the wrist than the ankle region. This compound elicited a positive oviposition response in gravid female *Ae. aegypti* mosquitoes [52]. Phenol was detected on more days and was more abundant in the ankle region. An antennal response for this compound has been noted [50]. Of interest is the detection of limonene on the ankle in a higher abundance, even though it was only detected in the ankle region on one day, as limonene is associated with individuals that are poorly attractive to mosquitoes [41]. All the compounds listed are plausible lead compounds in the development of mosquito attractants and repellents. Following up from this study an expanded study was completed where perceived mosquito attractiveness is assessed based on the skin chemical profiles of 20 volunteers providing an extended list of biological lead compounds to be used in vector control strategies [62].

3.3.3. Targeted analysis

Seventeen of the 19 target VOCs and semi-VOCs were unequivocally identified on the human skin using the selected reference standards, representing a broad range of chemical classes, and a passive sampling approach (refer to section 3.1). The presence of alcohols, aldehydes, carboxylic acids, esters, ketones, nitrogen containing compounds, and terpenes on the human skin surface was confirmed by means of the in-house constructed PDMS sampler loaded with authentic standards and GC×GC-TOFMS. To the authors' knowledge carvone and (*E*)-2-decenal have not previously been detected on the human skin. Carvone has previously been reported in human breath and (*E*)-2-decenal has been reported in human breast milk samples [8]. An exemplary contour plot showing four of the identified VOCs detected on the human wrist skin surface is given in Fig. 4.

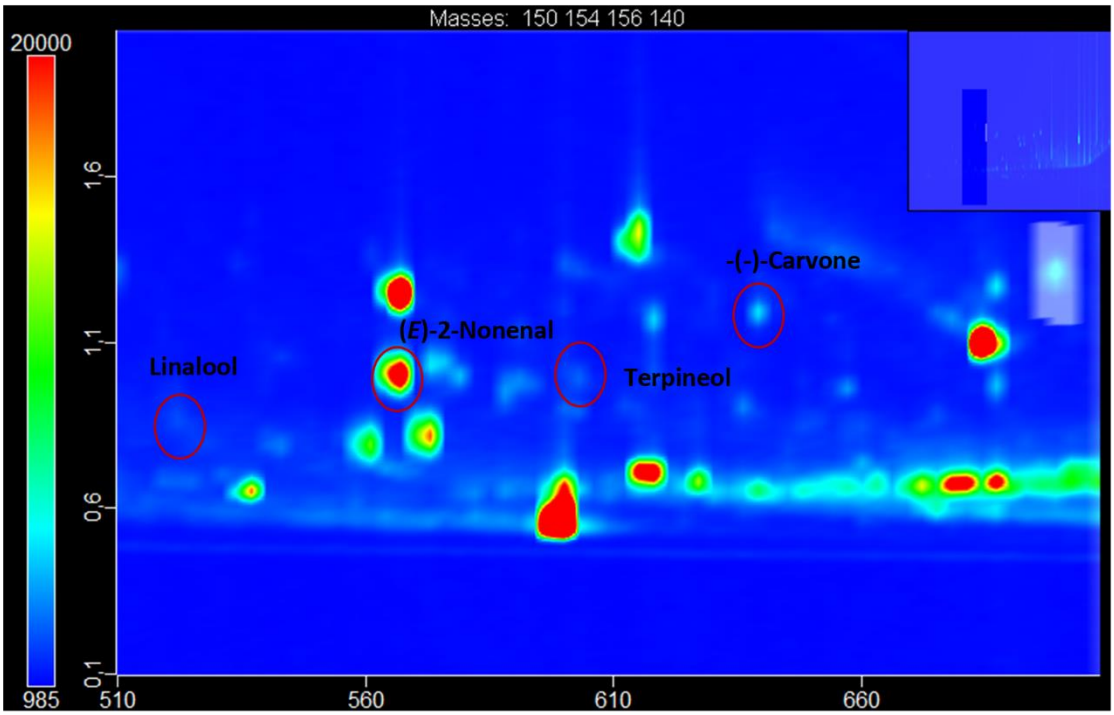

Figure 4. Contour plot of a reconstructed ion chromatogram (RIC) (GC×GC-TOFMS) of selected analytes collected from a human wrist sampled on Day 1. Target analytes detected are indicated. RIC: 140, 150, 154 and 156 *m/z*.

A box-and-whisker plot (Fig. 5) was used to investigate the differences between the wrist and ankle skin surface areas for the target analytes. Octanal, associated with highly mosquito attractive individuals [41], was more abundant on the ankle than wrist skin area. The same result was found for the aldehyde, nonanal. The mosquito plant attractant, terpineol [57] was also more abundant in the ankle region. 3-Methyl-2-butenal, tetradecanoic acid (refer to section 3.3.2) and 2-octanone (refer to section 3.3.2) were more abundant in the wrist area over the five days of sampling. Heptanal and butanoic acid, previously reported on skin [8], were not detected on the human skin surface during the sampling period, whilst propanoic acid, also previously reported to be present on the human skin surface [8, 15], was detected on Day 1 only. The large measurement variation in abundances of some of the compounds underpin the complexity of the human skin surface, specifically the skin surface microbiome. For example, octanal ranged from not detected on the wrist skin surface region (Day

1) to detection of a higher abundance on the wrist skin surface area on Day 4 compared to any of the abundances detected over five days of the ankle skin surface region sampling. 2-Octanone detected on the wrist skin surface area had the largest range in abundances of all the compounds (0.0330 – 3.0408 normalised TIC peak area) compared to, for example, indole detected on the wrist skin surface area with the smallest abundance range (0.0033 – 0.0080 normalised TIC peak area).

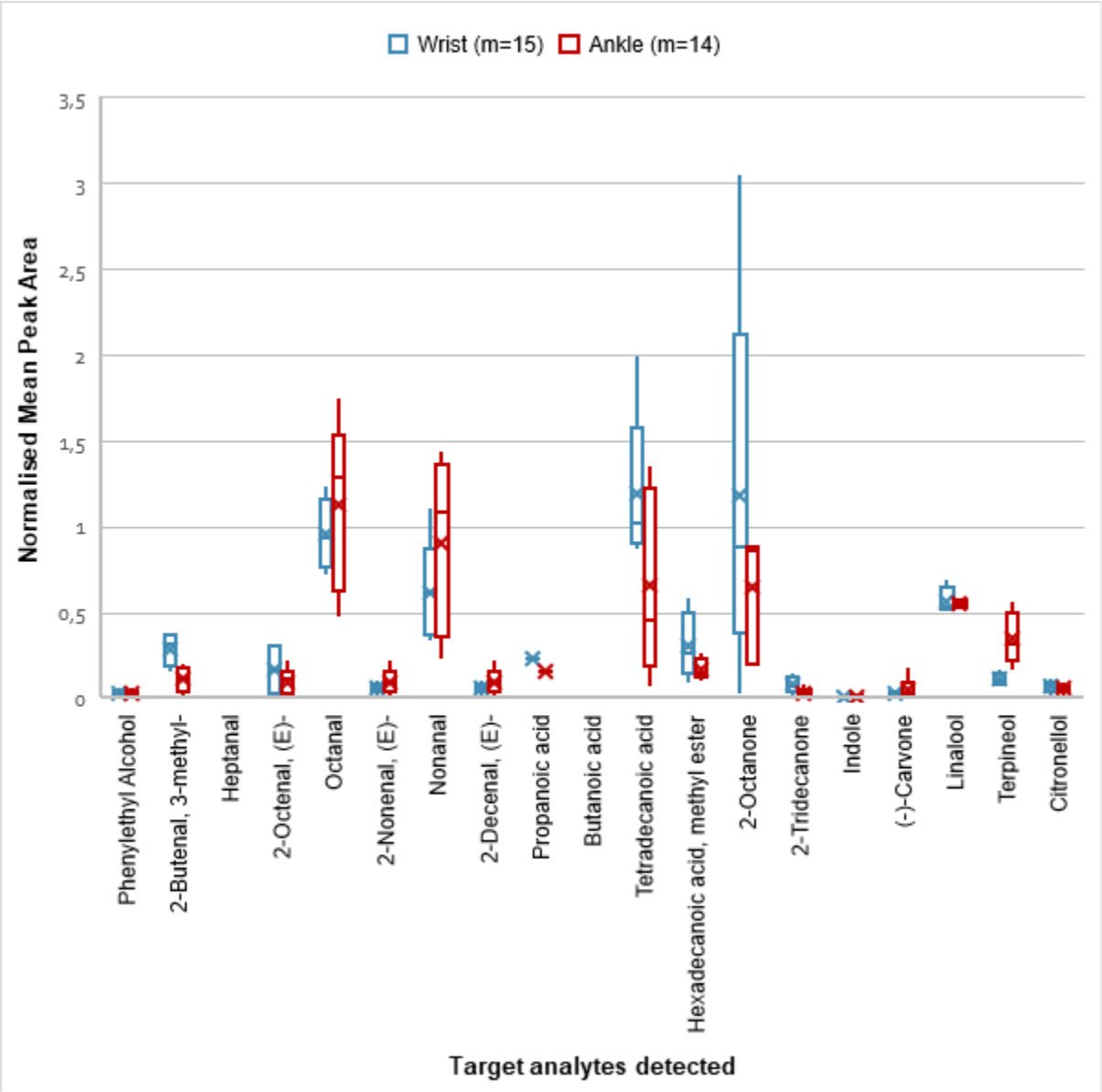

Figure 5: Box-and-whisker plot of the mean peak areas (wrists: m = 15; ankles: m=14) (TIC) of the 19 target analytes detected on the wrist (blue) and ankle (red) of a female volunteer during a five-day sampling period. Peak areas were normalised using the peak area (TIC) of the eucalyptol IS.

3.4. Concluding remarks

A non-invasive passive sampling method was used to detect a broad range of chemical compounds on the human skin surface from a single volunteer. The in-house developed PDMS mini-sampler, worn as a bracelet or an anklet, and followed by direct TD in the GC inlet liner with GC×GC-TOFMS provided an uncomplicated scheme to compare the chemical profiles of different human skin regions. Solvent modification of the PDMS sampler did not impede on the performance of the sampler and allowed for a simplified method for the addition of an internal standard to sorptive material thereby providing increased confidence in complex data set comparisons. The PDMS sampler is easy to make and to use, and it allows for human skin sampling that is comfortable for the volunteer and does not impede on the dignity of the individual sampled. Additionally, the method introduces a simple barrier, i.e. Mylar® reflective sheeting, to prevent atmospheric contamination of the PDMS sampler during sampling. The small size of the PDMS sampler permitted thermal desorption directly in the inlet liner of the GC, thus reducing sample introduction time and cryo-focussing was mostly not required. Thousands of chromatographic peaks resulting from compounds present on the human skin surface from one individual sampled consecutively over a five-day period were effectively separated when using GC×GC-TOFMS in combination with the PDMS passive sampler. This technique provided increased separation power and improved sensitivity for the detection of a broad range of chemical compounds down to pg levels. This approach facilitated the tentative identification of 46 previously unreported skin volatiles from a broad range of chemical classes, including alkenes, alcohols, ketones, ethers, aldehydes, and esters. The application of the passive sampling method to human skin surface samples allowed the detection of over 545 compounds which were narrowed down to 86 tentatively identified VOCs and semi-VOCs that contributed to the differences in the skin surface chemical profile of the ankle and wrist area. Seventeen compounds were unequivocally identified on the human skin surface with two compounds not previously reported on the human skin surface, namely carvone and (*E*)-2-decenal. Identification of chemical compounds that contributed to the differences in the two human surface skin regions sampled was achieved. Compounds that were closely associated with the wrist included 6-methyl-1-heptanol, 3-(4-isopropylphenyl)-2-

methylpropionaldehyde, 2-phenoxyethyl isobutyrate, and 2,4,6-trimethyl-pyridine. Conversely, compounds only detected on the ankle region included 2-butoxyethanol phosphate, 2-heptanone, and *p*-menthan-8-ol. Over 40 of the skin surface compounds detected are known mosquito semiochemicals, thus confirming the potential of using this method in the development of attractants and repellents in vector control applications.

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Supplementary Information

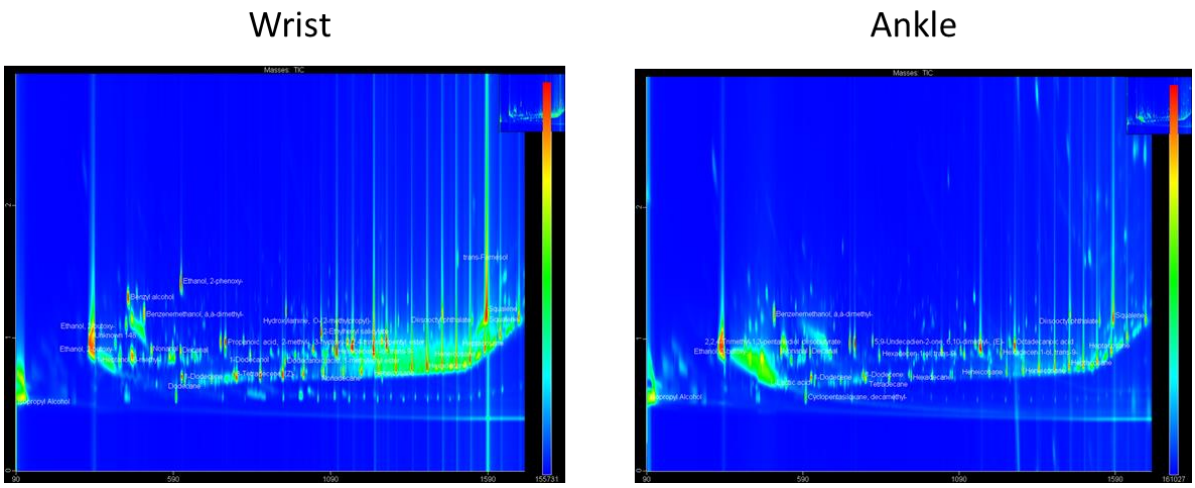

Figure S1. Contour plots (Total Ion Chromatogram - GC×GC-TOFMS) from the analysis of skin volatiles from a human volunteer using a non-invasive PDMS sampler. The contour plot on the left shows the chemical profile of the wrist skin surface region and the contour plot on the right is the chemical profile of the ankle skin surface region.

Table S1. Compounds tentatively identified using a spectral library match quality of ≥ 80% during the untargeted analysis of the human skin surface originating from the ankle and wrist skin surface areas sampled over a period of five days using an in-house developed PDMS sampler with inlet TD-GC×GC-TOFMS. Normalised mean peak areas (3 PDMS replicates per sampling period of 1 hour) are provided.

					WRIST					ANKLE				
					Normalised[c] Mean Peak Areas					Normalised Mean Peak Areas				
#	Compound	CAS Number	1D RT[a] (s)	2D RT[b] (s)	Day 1 (n=3)	Day 2 (n=3)	Day 3 (n=3)	Day 4 (n=3)	Day 5 (n=3)	Day 1 (n=2)[d]	Day 2 (n=3)	Day 3 (n=3)	Day 4 (n=3)	Day 5 (n=3)
Straight chain alkanes														
1	Butane	106-97-8	789	0.94	n.d[e]	n.d.	n.d.	n.d.	n.d.	n.d.	0.4290	n.d.	n.d.	n.d.
2	Nonane	111-84-2	342	0.63	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0356
3	Undecane	1120-21-4	537	0.66	n.d.	0.0212	0.0779	0.1166	0.0504	n.d.	0.0391	0.1401	0.4357	n.d.
4	Dodecane	112-40-3	627	0.68	0.0831	n.d.	0.4667	0.5616	0.4709	0.1812	0.2711	0.3190	0.4837	0.2923
5	Tridecane	629-50-5	711	0.69	0.0414	0.3337	0.2467	0.4010	0.4062	0.0822	0.1030	0.2609	0.4669	0.1146
6	Tetradecane	629-59-4	867	0.73	n.d.	0.4825	n.d.	0.5489	0.3294	0.0572	n.d.	n.d.	0.4903	n.d.
7	Pentadecane	629-62-9	1440	0.79	0.2993	0.2937	0.5759	1.6333	1.6554	0.2479	0.1265	0.2068	0.5394	1.0395
8	Hexadecane	544-76-3	864	0.71	1.4898	0.7310	0.5233	0.6667	0.6765	0.4675	0.2802	0.4921	0.6926	0.1561
9	Octadecane	593-45-3	1068	0.74	0.5414	0.7749	0.7880	1.2326	0.7846	0.3637	n.d.	0.5745	1.2984	1.0234
10	Nonadecane	629-92-5	1128	0.74	n.d.	0.4317	0.9201	0.9053	0.4398	0.1911	0.1358	0.0568	0.4995	0.2080
11	Eicosane	112-95-8	1317	0.73	0.3239	0.1461	0.4422	1.1641	0.4050	0.1965	0.9508	0.1783	0.4061	1.0682
12	Heneicosane	629-94-7	1185	0.74	2.7129	1.0448	0.1246	0.8384	0.6285	0.4483	0.2886	0.7470	0.8022	0.8531
13	Docosane	629-97-0	1296	0.75	n.d.	n.d.	2.4207	2.7199	2.1907	n.d.	n.d.	n.d.	1.2143	n.d.
14	Heptacosane	593-49-7	1578	0.92	n.d.	n.d.	n.d.	0.1161	0.4332	0.1513	n.d.	0.0229	n.d.	0.1588
15	Octacosane	630-02-4	1548	1.61	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.6396	n.d.	n.d.	n.d.
16	Hentriacontane	630-04-6	1443	0.88	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.6412
Branched chain alkanes														
17	Octane, 4-ethyl-	15869-86-0	588	0.65	n.d.	n.d.	0.0596	0.0679	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
18	Nonane, 2-methyl-	871-83-0	753	0.68	n.d.	n.d.	0.0191	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
19	Nonane, 3-methyl-	5911-04-6	690	0.66	n.d.	n.d.	n.d.	0.1944	0.2595	n.d.	n.d.	n.d.	n.d.	n.d.
20	Decane, 2-methyl-	6975-98-0	957	0.70	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0536	n.d.	n.d.	n.d.

21	Decane, 3-methyl-	13151-34-3	648	0.66	n.d.	n.d.	0.0133	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
22	Decane, 4-methyl-	2847-72-5	465	0.62	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2756	n.d.	n.d.
23	Undecane, 2-methyl-	7045-71-8	699	0.65	n.d.	n.d.	0.0197	n.d.	0.2133	n.d.	n.d.	0.1131	n.d.	n.d.
24	Undecane, 3-methyl-	1002-43-3	600	0.67	0.0195	n.d.	n.d.	n.d.	n.d.	n.d.	0.1997	n.d.	n.d.	n.d.
25	Dodecane, 2-methyl-	1560-97-0	681	0.68	n.d.	n.d.	n.d.	n.d.	0.4940	n.d.	n.d.	0.1666	n.d.	n.d.
26	Tridecane, 3-methyl-	6418-41-3	840	0.69	0.3001	0.3463	0.2878	0.4364	0.4195	0.1776	0.0886	0.0686	0.3352	0.2917
27	Tridecane, 4-methyl-	26730-12-1	687	0.69	n.d.	0.0043	n.d.	0.0629	n.d.	n.d.	n.d.	n.d.	n.d.	0.1007
28	Pentadecane, 2-methyl-	1560-93-6	912	0.70	0.2900	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
29	Hexadecane, 3-methyl-	6418-43-5	1431	0.77	n.d.	0.1888	n.d.	0.1836	0.1284	0.1296	0.1032	0.0621	0.0607	0.0779
30	Heptadecane, 2-methyl-	1560-89-0	1200	2.97	n.d.	0.1387	0.0751	n.d.	0.1092	n.d.	n.d.	n.d.	n.d.	0.1597
31	Heptadecane, 3-methyl-	6418-44-6	1050	0.72	n.d.	n.d.	n.d.	0.2115	n.d.	n.d.	n.d.	n.d.	n.d.	0.1298
32	Octadecane, 2-methyl-	1560-88-9	1107	0.73	0.0114	0.0949	0.4714	n.d.	0.1275	0.4255	0.1250	0.4969	0.1066	0.4306
33	Nonadecane, 2-methyl-	1560-86-7	1425	0.77	n.d.	0.3179	0.6422	0.0847	0.2585	0.3758	1.1122	n.d.	0.4372	0.1745
34	Eicosane, 2-methyl-	1560-84-5	1707	1.16	n.d.	n.d.	n.d.	0.1418	0.2449	n.d.	0.4621	n.d.	0.3429	0.8652
35	Heptane, 5-ethyl-2-methyl-	13475-78-0	465	0.63	0.4118	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
36	Octane, 3,5-dimethyl-	15869-93-9	1083	0.72	n.d.	n.d.	0.0692	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
37	Octane, 2,7-dimethyl-	1072-16-8	912	0.70	n.d.	n.d.	n.d.	1.7306	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
38	Decane, 3,7-dimethyl-	17312-54-8	1005	0.72	n.d.	n.d.	0.5643	n.d.	0.8910	n.d.	n.d.	0.2121	0.6751	0.4464
39	Decane, 2,9-dimethyl-	1002-17-1	819	0.69	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2508	n.d.
40	Undecane, 2,6-dimethyl-	17301-23-4	639	0.66	n.d.	0.0495	n.d.	0.0421	n.d.	n.d.	n.d.	n.d.	0.0180	0.1761
41	Heptadecane, 2,6-dimethyl-	54105-67-8	1395	0.75	n.d.	n.d.	n.d.	0.3013	0.0048	n.d.	0.6827	0.3777	0.0851	0.4913
42	Decane, 2,5,9-trimethyl-	62108-22-9	735	0.67	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2865	n.d.	n.d.	n.d.
43	Decane, 2,3,5,8-tetramethyl-	192823-15-7	762	0.69	0.1765	0.1394	n.d.	0.2892	n.d.	n.d.	n.d.	0.2234	n.d.	n.d.
44	Dodecane, 2,6,10-trimethyl-	3891-98-3	774	0.68	0.1919	n.d.	n.d.	n.d.	0.3392	0.1225	0.0758	0.1688	0.1213	0.1605
45	Dodecane, 2,7,10-trimethyl-	74645-98-0	1065	2.30	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.3992
46	Dodecane, 2,6,11-trimethyl-	31295-56-4	1011	0.69	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.8366
47	Pentadecane, 2,6,10-trimethyl-	3892-00-0	1551	0.86	n.d.	n.d.	n.d.	0.4899	n.d.	0.0919	0.0937	n.d.	n.d.	n.d.
48	Hexadecane, 2,6,10,14-tetramethyl-	638-36-8	1176	0.72	0.1339	n.d.	n.d.	1.8873	n.d.	0.0900	n.d.	n.d.	n.d.	0.7654
49	Heptadecane, 2,6,10,14-tetramethyl-	18344-37-1	1011	0.69	0.5650	0.7408	0.4864	1.6488	0.6279	0.0325	0.0773	0.0919	0.8381	0.3020
Non-aromatic cyclic hydrocarbons														
50	Pentane, 2-cyclopropyl-	5458-16-2	465	0.85	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	2.4681	n.d.	n.d.

51	Cyclohexane, (1-methylethyl)-	696-29-7	744	0.76	n.d.	0.0349	0.0893	n.d.	0.1060	0.0219	0.0361	0.0929	n.d.	0.2437
52	Cyclooctane, 1,4-dimethyl-, cis-	13151-99-0	1095	0.73	0.3351	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
53	Cyclooctane, 1,4-dimethyl-, trans-	13151-98-9	1251	0.78	n.d.	n.d.	0.1159	n.d.	n.d.	n.d.	0.2342	n.d.	n.d.	n.d.
54	Cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	1647	1.14	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.4202
55	Cyclooctane, 1,2-diethyl-	23609-46-3	1116	0.76	n.d.	0.1454	n.d.	n.d.	n.d.	0.3786	n.d.	n.d.	n.d.	n.d.
56	Cyclohexane, hexyl-	4292-75-5	657	0.76	n.d.	n.d.	n.d.	0.1468	n.d.	0.1004	n.d.	n.d.	n.d.	0.1026
57	Cyclopentane, 1-pentyl-2-propyl-	62199-51-3	1047	0.75	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.3741	n.d.	n.d.	n.d.
58	Cyclotetradecane	295-17-0	978	0.87	0.6030	0.6336	0.4819	0.9287	0.5706	n.d.	0.4103	0.3288	0.8228	0.7393
59	Cyclohexane, octyl-	1795-15-9	1626	1.14	0.1165	0.2100	n.d.	0.2101	0.1212	0.0169	0.1293	0.1170	0.0400	0.1786
60	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	645-10-3	1539	0.87	n.d.	n.d.	n.d.	2.3316	n.d.	n.d.	n.d.	n.d.	0.4179	n.d.
61	Cyclohexane, undecyl-	54105-66-7	1689	1.31	0.1811	n.d.	n.d.	0.1452	0.0245	0.1538	0.0794	n.d.	0.1877	n.d.
62	n-Heptadecylcyclohexane	19781-73-8	1575	1.00	0.1598	n.d.	0.2464	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
63	Cyclopentane, heneicosyl-	6703-82-8	1680	1.24	0.0629	0.1400	0.3641	0.1857	0.2269	0.1532	0.1011	0.5131	0.3156	0.4814
Non-cyclic alkenes														
64	2-Octene	111-67-1	243	0.62	n.d.	n.d.	0.0895	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
65	1-Nonene	124-11-8	330	0.65	0.0581	n.d.	n.d.	n.d.	n.d.	n.d.	0.1179	n.d.	n.d.	0.4681
66	3-Dodecene, (Z)-	7239-23-8	636	0.71	n.d.	n.d.	n.d.	0.4682	0.3783	n.d.	n.d.	n.d.	0.1386	0.2442
67	1-Dodecene	112-41-4	618	0.71	0.4899	n.d.	n.d.	0.2698	n.d.	n.d.	0.6097	n.d.	n.d.	2.1037
68	5-Dodecene, (E)-	7206-16-8	558	0.67	n.d.	n.d.	0.0149	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
69	2-Tridecene, (E)-	41446-58-6	1107	0.90	n.d.	0.1966	0.1304	n.d.	n.d.	n.d.	0.1013	n.d.	n.d.	0.0488
70	2-Tridecene, (Z)-	41446-59-7	852	0.73	n.d.	n.d.	n.d.	n.d.	0.4412	n.d.	0.1893	n.d.	n.d.	0.2784
71	5-Tridecene, (E)-	23051-84-5	663	0.71	n.d.	0.2188	0.0476	0.1712	0.2277	0.0274	0.0877	n.d.	0.3504	0.1572
72	3-Tetradecene, (E)-	41446-68-8	783	0.73	n.d.	1.0957	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.5287	n.d.
73	3-Tetradecene, (Z)-	41446-67-7	783	0.73	n.d.	n.d.	n.d.	n.d.	0.5056	n.d.	n.d.	n.d.	n.d.	n.d.
74	4-Tetradecene, (E)-	41446-78-0	969	0.72	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.3160	n.d.	n.d.
75	Cetene	629-73-2	858	0.73	0.3630	n.d.	0.2199	n.d.	n.d.	n.d.	0.1647	0.2369	0.1457	n.d.
76	7-Hexadecene, (Z)-	35507-09-6	930	0.74	n.d.	n.d.	n.d.	n.d.	0.0331	0.0024	n.d.	n.d.	0.1471	n.d.
77	8-Heptadecene	2579-04-6	1014	0.75	0.3110	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
78	5-Octadecene, (E)-	7206-21-5	1116	0.75	0.2015	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

79	1-Nonadecene	18435-45-5	1122	0.75	0.2681	0.1442	0.1433	0.5892	n.d.	n.d.	0.0947	0.0028	n.d.	0.4118
80	cis-2-Methyl-7-octadecene	35354-39-3	1029	0.75	n.d.	0.0600	0.1950	0.4040	n.d.	n.d.	n.d.	0.4342	0.1238	0.5212
81	10-Heneicosene (c,t)	95008-11-0	1302	0.79	0.2164	n.d.	0.4559	0.6277	0.2262	0.0651	n.d.	n.d.	0.6804	n.d.
82	1-Docosene	1599-67-3	1182	0.76	0.0885	0.1493	0.3597	0.2786	0.5752	0.0925	0.0545	0.1517	0.4499	0.4636
83	Nonacos-1-ene	18835-35-3	1644	1.12	n.d.	0.0384	0.2391	0.0738	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
84	1-Hexene, 3,5-dimethyl-	7423-69-0	1005	0.73	n.d.	n.d.	n.d.	n.d.	0.2364	n.d.	n.d.	n.d.	n.d.	0.6297
85	3,5-Octadiene, 2,7-dimethyl-, (Z,Z)-	28980-73-6	549	0.99	0.0182	n.d.	n.d.	0.1063	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
86	1-Octene, 3,7-dimethyl-	4984-01-4	240	0.62	n.d.	n.d.	n.d.	n.d.	0.3340	n.d.	0.8264	0.1638	0.3359	n.d.
87	2,4,6,8-Tetramethyl-1-undecene	59920-26-2	1227	0.91	n.d.	0.7703	n.d.	1.5809	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
88	1,3-Octadiene	1002-33-1	267	0.68	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1643	n.d.	n.d.	n.d.
89	1,13-Tetradecadiene	21964-49-8	1209	0.95	n.d.	n.d.	n.d.	n.d.	n.d.	0.0555	n.d.	n.d.	n.d.	n.d.
90	Squalene	111-02-4	1584	1.22	8.1246	1.7521	2.5912	0.6538	2.2557	2.3415	2.7405	2.6820	2.6337	2.8474
Cyclic alkenes														
91	1,4-Methanobenzocyclodecene, 1,2,3,4,4a,5,8,9,12,12a-decahydro-	74708-73-9	951	1.11	n.d.	n.d.	n.d.	0.0056	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Benzyl and phenyl hydrocarbons														
92	p-Xylene	106-42-3	297	0.84	n.d.	n.d.	n.d.	1.7533	2.0126	n.d.	n.d.	0.3847	0.1215	n.d.
93	o-Xylene	95-47-6	309	0.91	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.2063
94	Benzene, 1,3-dimethyl-	108-38-3	297	0.84	n.d.	n.d.	0.3266	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
95	Benzene, 1,2,3-trimethyl-	526-73-8	447	0.95	n.d.	0.0287	n.d.	n.d.	n.d.	n.d.	0.3798	n.d.	n.d.	n.d.
96	Benzene, 1-ethyl-3-methyl-	620-14-4	390	0.87	n.d.	n.d.	0.9308	2.1416	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
97	Benzene, (1-methylethyl)-	98-82-8	447	0.95	n.d.	n.d.	0.1018	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
98	(E)-1-Phenyl-1-butene	1005-64-7	555	1.04	n.d.	n.d.	n.d.	n.d.	0.0357	n.d.	n.d.	n.d.	0.1116	n.d.
99	o-Cymene	527-84-4	570	1.00	n.d.	n.d.	n.d.	n.d.	0.0498	n.d.	n.d.	0.1862	0.3141	0.3251
100	Benzene, 1-methyl-3-propyl-	1074-43-7	477	0.87	n.d.	n.d.	n.d.	0.0708	0.2048	n.d.	n.d.	n.d.	n.d.	n.d.
101	Benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	528	0.95	n.d.	n.d.	n.d.	0.2172	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
102	Benzene, 2-ethyl-1,4-dimethyl-	1758-88-9	501	0.91	n.d.	n.d.	n.d.	n.d.	0.1305	n.d.	0.6055	n.d.	n.d.	n.d.
103	Benzene, 1-methyl-4-(1-methylpropyl)-	1595-16-0	579	0.93	n.d.	0.0576	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
104	Benzene, 1,3-diethyl-5-methyl-	2050-24-0	612	0.96	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1282	n.d.	n.d.
105	Biphenyl	92-52-4	753	1.33	n.d.	n.d.	n.d.	n.d.	n.d.	0.0027	n.d.	0.0073	0.0021	0.0027
106	Benzene, 4-hexenyl-	23086-43-3	846	1.22	0.0008	0.0023	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

107	1,1'-Biphenyl, 4-methyl-	644-08-6	834	1.30	0.0019	0.0011	n.d.	n.d.	0.0007	n.d.	n.d.	0.0010	0.0020	0.0005
108	1,1'-Biphenyl, 2-methyl-	643-58-3	771	1.24	n.d.	n.d.	n.d.	n.d.	0.0002	0.0014	n.d.	n.d.	n.d.	n.d.
109	4,4'-Dimethylbiphenyl	613-33-2	909	1.26	0.0015	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
110	Benzene, (1-propylheptyl)-	4537-12-6	891	0.86	0.0279	0.0343	0.0119	0.0181	0.0209	0.0133	0.0108	0.0157	0.0045	0.0126
111	Benzene, (1-butylhexyl)-	4537-11-5	885	0.86	0.0201	0.0189	n.d.	0.0502	0.0382	0.0186	0.0208	0.0157	0.0080	n.d.
112	Benzene, (1-methylnonyl)-	4537-13-7	927	0.89	0.0795	n.d.	0.0597	n.d.	n.d.	n.d.	0.0737	0.0554	n.d.	n.d.
113	Benzene, (1-propyloctyl)-	4536-86-1	960	0.87	0.0652	n.d.	0.0512	0.0767	0.0681	0.0316	0.0411	0.0502	0.0594	0.0521
114	Benzene, (1-methyldecyl)-	4536-88-3	999	0.89	0.0846	0.0908	0.0666	n.d.	0.1026	0.0494	0.0657	0.0528	0.0937	0.0718
115	Benzene, (1-pentylhexyl)-	4537-14-8	951	0.86	n.d.	0.1957	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
116	Benzene, (1-butylheptyl)-	4537-15-9	954	0.86	n.d.	n.d.	0.0940	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0850
117	Benzene, (1-ethylnonyl)-	4536-87-2	972	0.88	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0323
118	Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-	1889-67-4	1062	1.30	0.0022	0.0098	n.d.	0.0012	0.0010	0.0018	0.0016	n.d.	n.d.	0.0009
119	Benzene, (1-propylnonyl)-	2719-64-4	1026	0.87	0.0704	0.0878	0.1143	0.1222	0.0944	0.0474	0.0556	0.0700	0.0781	0.0688
120	Benzene, (1-pentylheptyl)-	2719-62-2	1017	0.86	0.1683	0.2284	0.1693	n.d.	n.d.	n.d.	0.1450	0.1578	n.d.	n.d.
121	Benzene, (1-butyloctyl)-	2719-63-3	1017	0.86	n.d.	n.d.	n.d.	0.2548	0.2530	n.d.	0.1580	n.d.	0.2120	0.1773
122	Benzene, (1-propyldecyl)-	4534-51-4	1089	0.87	0.1488	0.1277	n.d.	0.1979	0.1111	0.0461	0.0789	0.0681	0.0873	0.1191
123	Benzene, (1-pentyloctyl)-	4534-49-0	1077	0.86	n.d.	n.d.	0.6773	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Cyclic aromatic hydrocarbons														
124	1H-Indene, 2,3-dihydro-4,7-dimethyl-	6682-71-9	666	1.10	n.d.	n.d.	n.d.	n.d.	0.0036	0.0337	n.d.	n.d.	n.d.	0.0759
Poly aromatic hydrocarbons (PAHs)														
125	Triacetin	102-76-1	717	1.24	n.d.	0.0166	0.0062	0.0123	0.0082	0.0100	0.0134	0.0135	0.0180	0.0177
126	Azulene	275-51-4	591	1.30	n.d.	n.d.	n.d.	0.0532	0.0545	0.0636	0.0695	n.d.	0.0946	0.0859
127	Acenaphthene	83-32-9	831	1.47	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0006	n.d.	n.d.
128	Fluorene	86-73-7	903	1.49	n.d.	n.d.	0.0267	n.d.	n.d.	n.d.	n.d.	0.0130	n.d.	n.d.
129	9H-Xanthene	92-83-1	942	1.40	n.d.	n.d.	n.d.	n.d.	0.0000	n.d.	n.d.	n.d.	n.d.	n.d.
130	Phenanthrene	85-01-8	1032	1.71	n.d.	n.d.	n.d.	0.0047	0.0086	0.0038	0.0080	0.0078	0.0304	0.0239
131	Naphthalene, 1,2,3,4-tetrahydro-	119-64-2	573	1.12	n.d.	n.d.	n.d.	0.0174	n.d.	n.d.	n.d.	n.d.	0.0175	n.d.
132	Naphthalene, 1-methyl-	90-12-0	687	1.27	0.0139	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
133	Naphthalene, 2-methoxy-	93-04-9	807	1.44	0.0031	0.0019	n.d.	0.0005	0.0005	0.0025	0.0012	0.0011	n.d.	0.0015

134	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	2809-64-5	687	1.16	0.0859	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
135	Bicyclo[4,4,1]undeca-1,3,5,7,9-pentaene	2443-46-1	699	1.32	n.d.	n.d.	n.d.	0.0032	0.0005	n.d.	n.d.	n.d.	0.0091	0.0116
136	2-Naphthyl methyl ketone	93-08-3	918	1.65	n.d.	0.0032	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
137	Naphthalene, 2,6-dimethyl-	581-42-0	777	1.24	n.d.	n.d.	n.d.	0.0027	0.0011	n.d.	n.d.	n.d.	0.0015	0.0044
138	Naphthalene, 1-ethyl-	1127-76-0	768	1.25	0.0008	0.0004	n.d.	0.0009	0.0004	0.0007	n.d.	n.d.	n.d.	n.d.
139	Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	4175-54-6	732	1.10	n.d.	n.d.	0.0018	n.d.	n.d.	0.0031	n.d.	0.0023	n.d.	n.d.
140	Naphthalene, 1,2,3,4-tetrahydro-2,7-dimethyl-	13065-07-1	732	1.10	n.d.	n.d.	n.d.	n.d.	0.0112	n.d.	n.d.	n.d.	n.d.	n.d.
141	Naphthalene, 1,4,5-trimethyl-	2131-41-1	873	1.24	0.0167	n.d.	n.d.	0.0006	n.d.	n.d.	0.0007	n.d.	0.0006	0.0091
142	Naphthalene, 2-(1-methylethyl)-	2027-17-0	864	1.26	n.d.	0.0016	n.d.	0.0028	n.d.	0.0021	n.d.	n.d.	0.0030	n.d.
143	Naphthalene, 1,4,6-trimethyl-	2131-42-2	873	1.24	n.d.	n.d.	n.d.	0.0098	0.0060	n.d.	n.d.	0.0001	n.d.	n.d.
144	Naphthalene, 1,2,3-trimethyl-4-propenyl-, (E)-	26137-53-1	990	1.30	0.0181	0.0134	0.0103	0.0150	0.0102	0.0125	0.0123	0.0091	0.0251	0.0157
145	2,6-Diisopropylnaphthalene	24157-81-1	978	1.13	0.1789	0.1207	0.0513	0.1624	0.0715	0.0891	0.0799	0.0211	0.1231	0.0927
146	Naphthalene, 1-(phenylmethoxy)-	607-58-9	1248	1.76	0.0523	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
147	Octadecahydro-benzo[cd]pyrene	0-00-0	1188	1.15	0.0174	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0264
Alcohols														
148	Isopropyl Alcohol	67-63-0	90	0.52	0.8161	0.6759	n.d.	0.9495	0.6506	1.2604	0.1984	0.0280	0.6971	0.5916
149	1-Octanol	111-87-5	495	0.86	0.1932	0.3415	0.2512	0.3796	0.3763	0.6509	0.3552	0.5112	1.2960	n.d.
150	2-Nonanol	628-99-9	540	0.68	n.d.	n.d.	0.1154	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
151	1-Nonanol	143-08-8	552	0.83	n.d.	n.d.	n.d.	0.5441	0.3103	0.0663	0.1673	n.d.	0.5949	1.0670
152	1-Dodecanol	112-53-8	834	0.88	0.6177	n.d.	n.d.	n.d.	n.d.	n.d.	0.2689	0.4508	n.d.	n.d.
153	n-Tridecan-1-ol	112-70-9	909	0.87	n.d.	n.d.	0.4510	0.4122	0.6660	0.2906	0.1108	0.0174	0.0959	0.0983
154	3-Tetradecanol	1653-32-3	927	0.83	n.d.	n.d.	n.d.	0.1597	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
155	1-Hexadecanol	36653-82-4	1119	0.86	2.2567	1.4447	0.6240	2.1106	n.d.	n.d.	n.d.	n.d.	0.9857	n.d.
156	1-Eicosanol	629-96-9	1497	0.84	0.1198	0.3151	0.2017	0.2479	0.4249	0.1018	0.1920	0.2023	0.3327	0.2015
157	5-Methyl-1-heptanol	7212-53-5	468	0.86	0.8674	n.d.	0.4121	n.d.	1.1604	n.d.	0.8355	n.d.	n.d.	n.d.
158	1-Heptanol, 6-methyl-	1653-40-3	420	0.83	1.8533	2.0528	0.7300	1.6999	1.3533	0.1238	1.8479	n.d.	n.d.	n.d.

159	1-Octanol, 3,7-dimethyl-	106-21-8	807	0.85	n.d.	0.4548	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
160	1-Hexanol, 3,5,5-trimethyl-	3452-97-9	513	0.83	0.3091	0.4724	0.2543	0.2716	0.2772	n.d.	0.2210	n.d.	n.d.	n.d.
161	trans-Geranylgeraniol	24034-73-9	1491	1.10	0.2902	0.2904	0.8105	0.4591	0.3243	0.0177	0.0059	0.0818	0.1409	0.0813
162	Cyclopropyl carbinol	2516-33-8	480	1.97	0.0029	0.1671	0.0207	0.1559	0.0873	0.1441	0.5488	0.1108	0.1705	1.9970
163	Cyclohexanol, 1-methyl-4-(1-methylethyl)-	21129-27-1	588	0.94	0.3021	n.d.	n.d.	0.1518	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
164	Patchouli alcohol	5986-55-0	969	1.18	n.d.	n.d.	n.d.	0.1291	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
165	Cholesterol	57-88-5	1281	0.10	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.9082	0.4486	2.0100
166	Hexadecen-1-ol, trans-9-	64437-47-4	1107	0.90	1.9459	n.d.	0.1697	n.d.	n.d.	0.3278	0.2599	0.4186	n.d.	0.7927
167	1,2-Ethanediol	107-21-1	156	0.91	n.d.	n.d.	n.d.	0.1971	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
168	Propylene Glycol	57-55-6	177	0.94	0.0103	n.d.	n.d.	n.d.	n.d.	0.3450	0.1318	0.1311	n.d.	n.d.
169	R-(-)-1,2-propanediol	4254-14-2	159	0.99	n.d.	1.3755	0.4827	n.d.	0.3177	n.d.	0.0071	0.2259	0.6858	1.5460
170	Glycerin	56-81-5	492	1.06	0.6071	1.6083	0.8787	1.3273	1.0834	0.9947	1.4565	1.4181	3.4020	3.3852
171	1,3-Butanediol, (S)-	24621-61-2	291	1.10	0.2318	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
172	1,3-Butanediol	107-88-0	297	1.07	n.d.	0.4127	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
173	2,3-Butanediol, [S-(R*,R*)]-	19132-06-0	249	0.84	n.d.	0.2123	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
174	2,3-Butanediol	513-85-9	234	0.92	n.d.	n.d.	0.2346	0.1419	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
175	1,2-Pentanediol	5343-92-0	360	1.05	0.5519	1.2788	n.d.	2.0260	0.9334	n.d.	n.d.	n.d.	0.4774	0.5538
176	1-Propanol, 2,2'-oxybis-	108-61-2	465	1.09	n.d.	n.d.	n.d.	n.d.	0.6306	n.d.	n.d.	0.2599	n.d.	n.d.
177	1,3-Pentanediol, 2,2,4-trimethyl-	144-19-4	558	1.07	0.0416	0.0297	n.d.	0.1554	0.0672	n.d.	n.d.	n.d.	0.2000	0.1799
178	2,4,7,9-Tetramethyl-5-decyn-4,7-diol	126-86-3	789	0.89	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.6414	n.d.	n.d.	0.2405
179	β-D-Glucopyranose, 1,6-anhydro-	498-07-7	762	2.60	0.0118	0.0087	n.d.	n.d.	0.0380	n.d.	0.0241	n.d.	n.d.	n.d.
180	Isosorbide	652-67-5	687	1.53	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0102	n.d.	n.d.
181	Ethanol, 2,2'-oxybis-	111-46-6	390	1.27	0.0117	n.d.	n.d.	0.0900	0.0176	n.d.	0.0989	0.0826	0.1728	n.d.
182	Ethanol, 2-(2-methoxyethoxy)-	111-77-3	357	1.11	0.0972	0.3423	n.d.	0.6004	n.d.	n.d.	n.d.	n.d.	n.d.	0.2632
183	Ethanol, 2-butoxy-	111-76-2	327	1.05	n.d.	n.d.	n.d.	n.d.	n.d.	2.0607	0.8985	n.d.	0.6312	n.d.
184	2-Propanol, 1,1'-oxybis-	110-98-5	441	1.11	0.6187	0.3117	0.3566	1.6301	0.3128	0.3392	0.2189	n.d.	0.9812	1.2434
185	1-Propanol, 2-(2-hydroxypropoxy)-	106-62-7	486	1.17	0.1574	0.6308	0.3489	1.5692	n.d.	0.2434	n.d.	n.d.	n.d.	n.d.
186	Ethanol, 2-(2-ethoxyethoxy)-	111-90-0	420	1.10	0.0187	0.4215	0.4650	0.4275	0.4926	n.d.	0.3749	0.2857	0.9046	n.d.
187	Triethylene glycol	112-27-6	630	1.36	0.0093	n.d.	0.0095	0.0244	n.d.	n.d.	0.0380	0.1499	0.2225	0.2837
188	Ethanol, 2-(2-butoxyethoxy)-	112-34-5	594	1.06	0.1478	0.2095	0.1452	0.3728	0.2783	0.3393	0.3955	0.3207	0.5571	0.4056

189	Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	143-22-6	816	1.16	0.0018	0.0021	n.d.	0.0022	0.0029	0.0009	n.d.	n.d.	n.d.	n.d.
190	Ethanol, 2-(dodecyloxy)-	4536-30-5	1002	0.91	0.1047	n.d.	0.4012	0.2806	0.3728	0.1070	0.0983	0.1506	0.2999	0.1829
191	Diethylene glycol monododecyl ether	3055-93-4	1167	1.00	0.2035	0.1181	n.d.	0.1961	n.d.	0.0684	0.0399	0.0692	0.1236	0.1688
192	Triethylene glycol monododecyl ether	3055-94-5	1314	1.09	n.d.	0.0211	0.0252	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
193	Phenol	108-95-2	405	1.11	n.d.	0.0712	0.3716	0.1714	0.2643	0.8466	0.7130	n.d.	0.6045	1.7513
194	Benzyl alcohol	100-51-6	447	1.31	0.7186	0.0429	n.d.	0.3132	0.1694	0.0299	n.d.	0.0405	0.1939	0.0911
195	Phenol, 2-methyl-	95-48-7	477	1.12	n.d.	0.4117	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
196	Benzenemethanol, 4-methyl-	589-18-4	543	1.26	n.d.	0.0140	0.0111	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
197	Benzenemethanol, 2-methyl-	89-95-2	549	1.30	n.d.	0.0211	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
198	Phenylethyl Alcohol	60-12-8	522	1.30	n.d.	n.d.	0.0352	0.0347	n.d.	0.0109	n.d.	0.0332	0.0445	n.d.
199	Benzenemethanol, α,α-dimethyl-	617-94-7	498	1.18	n.d.	0.0465	n.d.	0.2085	n.d.	n.d.	n.d.	n.d.	n.d.	0.5245
200	Phenol, 2-methyl-5-(1-methylethyl)-	499-75-2	684	1.10	0.0868	0.0280	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
201	Phenol, 4-(1,1-dimethylpropyl)-	80-46-6	1020	1.13	n.d.	n.d.	0.0308	n.d.	n.d.	n.d.	n.d.	0.0119	n.d.	n.d.
202	Butylated Hydroxytoluene	128-37-0	861	0.99	0.0352	0.0755	0.0469	0.0454	0.0317	0.0091	0.0198	0.0180	0.0301	0.0219
203	Ethanol, 2-phenoxy-	122-99-6	615	1.43	1.0005	0.2359	0.1714	1.1704	0.1517	n.d.	0.0717	0.0295	0.3123	0.0609
204	3-Ethyl-4-methylpentan-1-ol	38514-13-5	447	0.87	0.1335	0.3639	n.d.	n.d.	0.4556	n.d.	n.d.	n.d.	n.d.	n.d.
205	1-Heptanol, 4-methyl-	817-91-4	456	0.88	n.d.	n.d.	0.5556	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
206	1-Pentanol, 2-ethyl-4-methyl-	106-67-2	711	0.72	n.d.	n.d.	0.3639	0.6214	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
207	1-Octanol, 2-butyl-	3913-02-8	786	0.83	n.d.	0.0608	n.d.	n.d.	0.2354	n.d.	n.d.	n.d.	0.1885	n.d.
208	2-Ethyl-1-dodecanol	19780-33-7	1068	0.77	0.9253	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
209	1-Decanol, 2-hexyl-	2425-77-6	1464	1.92	n.d.	n.d.	0.2626	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
210	4-Penten-2-ol	625-31-0	534	0.62	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.5019	0.2384	n.d.
211	2-Decen-1-ol	22104-80-9	582	0.89	n.d.	n.d.	n.d.	n.d.	0.5622	n.d.	n.d.	n.d.	n.d.	n.d.
212	11-Hexadecen-1-ol, (Z)-	56683-54-6	1317	0.94	n.d.	n.d.	n.d.	0.4217	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
213	7-Octen-2-ol, 2,6-dimethyl-	18479-58-8	498	0.83	0.1441	n.d.	n.d.	n.d.	0.2615	n.d.	0.1482	n.d.	n.d.	n.d.
214	1,6,10,14,18,22-Tetracosahexaen-3-ol, 2,6,10,15,19,23-hexamethyl-, (all-E)-(ñ)-	97232-74-1	1680	1.70	n.d.	0.0383	0.0745	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Terpenes														
215	Linalool	78-70-6	522	0.88	0.7713	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
216	Citronellol	106-22-9	636	0.93	n.d.	n.d.	0.0497	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

217	Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)-	5989-54-8	462	0.79	0.1740	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
218	D-Limonene	5989-27-5	462	0.79	n.d.	0.2007	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
219	Carvone	6485-40-1	639	1.19	0.0211	0.0261	0.0256	0.0319	0.0368	n.d.	n.d.	n.d.	n.d.	n.d.
220	Terpineol	0-00-0	603	1.01	n.d.	n.d.	n.d.	n.d.	n.d.	0.3063	0.3971	0.2173	0.5489	0.3106
221	Levomenthol	2216-51-5	588	0.94	n.d.	n.d.	0.0851	n.d.	n.d.	n.d.	n.d.	n.d.	0.1172	n.d.
222	Cyclohexanemethanol, α,α,4-trimethyl-	498-81-7	564	0.91	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0933	n.d.	0.1873	0.3837
223	Bicyclo[2,2,1]heptan-2-one, 1,7,7-trimethyl-, (1S)-	464-48-2	555	1.11	0.0252	n.d.	n.d.	0.1070	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
224	trans-β-Ionone	79-77-6	840	1.07	0.0243	0.0219	0.0114	n.d.	n.d.	0.0070	n.d.	n.d.	n.d.	n.d.
Ethers														
225	Diphenyl ether	101-84-8	768	1.33	0.0075	0.0101	0.0034	n.d.	0.0071	n.d.	0.0143	0.0070	0.0405	n.d.
226	Octane, 1,1'-oxybis-	629-82-3	975	0.77	0.0493	0.1468	0.1364	0.2028	0.1849	0.0564	0.0687	0.0567	0.1629	0.0937
227	Benzaldehyde, 4-methoxy-	123-11-5	639	1.55	0.0087	0.0088	0.0029	0.0072	0.0043	0.0043	0.0024	0.0014	0.0017	0.0060
228	Vanillin	121-33-5	756	1.66	0.0012	0.0104	0.0009	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
229	Estragole	140-67-0	603	1.12	0.0060	0.0156	n.d.	0.0266	0.0208	n.d.	0.2239	0.1315	0.1223	n.d.
230	2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	5466-77-3	1335	1.30	0.1060	0.1644	0.4799	0.2056	0.2351	0.0174	0.0424	0.0596	0.1682	0.1686
231	Safrole	94-59-7	681	1.22	n.d.	n.d.	n.d.	0.0540	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
232	Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-	104-66-5	1044	1.51	0.0138	0.0159	0.0246	0.0186	0.0132	0.0110	0.0168	0.0075	0.0230	0.0096
233	Ethylene oxide	75-21-8	858	0.66	n.d.	n.d.	0.0245	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
234	Oxirane, tetradecyl-	7320-37-8	1524	0.88	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.3208
235	Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentamethyl-3,7,11,15,19-heneicosapentaenyl)-, (all-E)-	7200-26-2	1641	1.46	0.2521	0.1616	0.4204	0.4418	0.1795	0.0846	0.0633	0.1037	0.1637	0.1020
236	2-Furanmethanol	98-00-0	285	1.04	0.0096	n.d.	0.2466	n.d.	n.d.	n.d.	0.2100	n.d.	n.d.	n.d.
237	2-Furancarboxaldehyde, 5-methyl-	620-02-0	378	1.30	n.d.	n.d.	n.d.	0.0368	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
238	Furan, 2-pentyl-	3777-69-3	420	0.81	0.6587	n.d.	0.3036	n.d.	n.d.	n.d.	0.4775	n.d.	n.d.	n.d.
239	Dibenzofuran	132-64-9	858	1.43	n.d.	n.d.	n.d.	0.0014	n.d.	0.0021	0.0027	0.0015	n.d.	n.d.

Aldehydes

240	Acetaldehyde	75-07-0	99	2.09	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0820
241	Hexanal	66-25-1	222	0.84	n.d.	n.d.	n.d.	0.0986	0.2966	0.0264	0.2581	n.d.	0.1860	0.6194
242	Octanal	124-13-0	423	0.90	0.2993	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
243	Nonanal	124-19-6	519	0.92	n.d.	0.1502	0.3839	n.d.	0.2501	n.d.	0.1701	0.1280	n.d.	1.3264
244	Decanal	112-31-2	612	0.91	0.3725	0.4631	0.7275	n.d.	n.d.	0.3968	0.1367	0.2559	0.4586	0.2749
245	Undecanal	112-44-7	699	0.90	0.1140	n.d.	0.1247	0.2554	0.1930	n.d.	0.1057	0.1325	0.1846	0.2803
246	Dodecanal	112-54-9	780	0.89	0.0675	n.d.	n.d.	0.2103	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
247	2-Nonenal, (E)-	18829-56-6	567	0.98	0.0407	0.0239	0.0755	0.0927	0.0560	n.d.	n.d.	n.d.	n.d.	n.d.
248	2-Nonenal, (Z)-	60784-31-8	567	0.98	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0253	n.d.	n.d.	n.d.
249	2-Decenal, (E)-	3913-81-3	744	0.95	n.d.	n.d.	n.d.	n.d.	0.0745	n.d.	n.d.	n.d.	n.d.	n.d.
250	2-Undecenal	2463-77-6	744	0.95	n.d.	n.d.	n.d.	n.d.	0.1102	n.d.	n.d.	n.d.	n.d.	n.d.
251	2-Dodecenal, (E)-	20407-84-5	822	0.95	0.0155	n.d.	0.0323	0.0527	0.0201	n.d.	n.d.	n.d.	0.0065	0.0234
252	2-Butenal, 3-methyl-	107-86-8	207	0.99	0.1798	0.1737	0.3836	0.3410	0.2770	n.d.	n.d.	n.d.	n.d.	n.d.
253	2-Pentenal, 2-methyl-	623-36-9	258	0.89	0.0109	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
254	2,4-Nonadienal, (E,E)-	5910-87-2	615	1.07	0.0016	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
255	2,6-Octadienal, 3,7-dimethyl-, (E)-	141-27-5	663	1.07	0.0152	0.0199	0.0461	0.0350	0.0226	0.0257	0.0202	0.2458	n.d.	0.0592
256	2,4-Decadienal	2363-88-4	702	1.05	0.0047	n.d.	n.d.	0.0111	n.d.	n.d.	0.0023	0.0031	0.0055	n.d.
257	Isophthalaldehyde	626-19-7	612	1.85	0.0016	0.0004	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
258	Acetaldehyde, methoxy-	10312-83-1	96	0.50	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0105	n.d.	n.d.	n.d.
259	Benzaldehyde	100-52-7	372	1.28	n.d.	n.d.	n.d.	0.1291	0.0177	0.0028	0.0232	0.0472	0.1723	0.1505
260	Benzaldehyde, 4-methyl-	104-87-0	489	1.30	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0515	n.d.	n.d.	n.d.
261	Benzaldehyde, 3-methyl-	620-23-5	477	1.28	0.1070	n.d.	0.2858	n.d.	0.2323	n.d.	n.d.	n.d.	n.d.	0.0828
262	Benzeneacetaldehyde	122-78-1	450	1.36	n.d.	n.d.	0.0484	0.0511	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
263	Piperonal	120-57-0	705	1.65	0.0122	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
264	2,6-Dimethylbenzaldehyde	1123-56-4	579	1.26	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0204	0.0211	n.d.	n.d.
265	Cinnamaldehyde, (E)-	14371-10-9	654	1.51	0.0018	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
266	Benzaldehyde, 4-propyl-	28785-06-0	663	1.23	0.0052	n.d.	0.0223	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
267	4-(t-Butyl)benzaldehyde	939-97-9	696	1.18	0.0018	n.d.	n.d.	0.0048	0.0023	n.d.	n.d.	n.d.	n.d.	n.d.
268	3-(4-Isopropylphenyl)-2-methylpropionaldehyde	103-95-7	813	1.19	n.d.	n.d.	n.d.	0.0171	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

269	Lilial	80-54-6	864	1.17	0.0156	n.d.	0.0177	0.1194	n.d.	0.0093	n.d.	n.d.	n.d.	n.d.
270	Octanal, 2-(phenylmethylene)-	101-86-0	1014	1.19	0.0729	0.0480	0.1135	0.1163	0.1449	0.0228	0.0234	0.0409	0.0416	0.0466
271	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	1620-98-0	1026	1.24	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0016	n.d.	n.d.
Ketones														
272	2-Heptanone	110-43-0	312	0.87	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.5736	n.d.
273	2-Octanone	111-13-7	414	0.88	0.1187	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
274	2-Decanone	693-54-9	603	0.90	n.d.	0.0173	0.0213	0.0415	n.d.	n.d.	n.d.	n.d.	0.1444	n.d.
275	2-Undecanone	112-12-9	690	0.89	n.d.	n.d.	0.0584	0.1169	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
276	2-Dodecanone	6175-49-1	771	0.89	0.0637	0.1210	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0766	n.d.
277	3-Dodecanone	1534-27-6	768	0.88	0.0962	0.1372	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
278	2-Tridecanone	593-08-8	849	0.89	0.1262	0.1549	0.0525	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
279	3-Tridecanone	1534-26-5	843	0.88	0.1012	0.1409	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
280	Cyclohexanone	108-94-1	309	1.16	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0171
281	Methyl glyoxal	78-98-8	120	0.61	n.d.	n.d.	n.d.	1.4214	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
282	Avobenzone	70356-09-1	1545	2.01	0.1527	n.d.	n.d.	n.d.	0.0521	n.d.	n.d.	n.d.	n.d.	n.d.
283	Acetophenone	98-86-2	474	1.35	0.0507	0.1230	0.1528	0.1782	0.2041	n.d.	0.0758	0.1143	n.d.	0.2207
284	2-Butanone, 4-(4-hydroxyphenyl)-	5471-51-2	873	1.61	0.0302	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
285	Benzophenone	119-61-9	927	1.61	0.0483	0.0524	0.0442	0.0402	0.0504	0.0258	0.0345	0.0225	0.0523	0.0350
286	1-(4-tert-Butylphenyl)propan-2-one	81561-77-5	804	1.22	0.0044	0.0072	0.0081	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
287	Methanone, (1-hydroxycyclohexyl)phenyl-	947-19-3	972	1.49	0.0027	0.0023	0.0021	0.0023	n.d.	0.0028	0.0033	n.d.	0.0039	0.0021
288	7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	88-29-9	1086	1.17	0.0371	0.0663	0.3000	0.0122	0.1144	0.0091	0.0176	0.0126	0.1340	0.0391
289	Maltol	118-71-8	525	1.39	n.d.	n.d.	0.0034	0.0028	n.d.	0.0031	0.0029	n.d.	0.0048	0.0036
290	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	82304-66-3	1116	1.25	0.0164	n.d.	n.d.	n.d.	n.d.	n.d.	0.0133	n.d.	n.d.	n.d.
291	6-Methyl-3,5-heptadiene-2-one	1604-28-0	516	1.12	0.0133	n.d.	0.1078	0.1801	0.0569	n.d.	0.0268	0.0728	0.0369	0.0228
292	5-Hepten-2-one, 6-methyl-	110-93-0	405	0.97	0.3406	0.3927	0.7212	1.4961	1.1251	0.8420	0.6956	n.d.	1.5848	1.0477
293	Ethanone, 1-(6,6-dimethylbicyclo[3,1,0]hex-2-en-2-yl)-	24555-40-6	840	0.98	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0067	0.0006

294	3,5,9-Undecatrien-2-one, 6,10-dimethyl-	141-10-6	906	1.08	0.0064	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
295	3,5,9-Undecatrien-2-one, 6,10-dimethyl-, (E,E)-	3548-78-5	906	1.08	n.d.	n.d.	0.0123	n.d.	n.d.	n.d.	n.d.	n.d.	0.0074	n.d.
296	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	3796-70-1	813	0.98	0.2523	0.2107	0.1177	n.d.	n.d.	0.2521	0.2300	0.1590	n.d.	0.2275
297	α-Isomethyl ionone	127-51-5	840	0.98	0.0238	n.d.	n.d.	n.d.	n.d.	0.0154	0.0123	0.0486	n.d.	n.d.
298	2-Propanone, 1-methoxy-	5878-19-3	99	0.52	0.6323	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.5731	0.4177
299	Furyl hydroxymethyl ketone	17678-19-2	495	1.39	0.0080	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
300	Levoglucosenone	37112-31-5	501	1.79	0.0095	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
301	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	28564-83-2	552	1.30	n.d.	n.d.	0.0208	0.0413	0.0558	n.d.	0.1303	0.0319	0.0534	0.0910
302	2-Pentanone, 4-hydroxy-4-methyl-	123-42-2	315	0.86	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.7920	n.d.
303	1H-Inden-1-one, 2,3-dihydro-	83-33-0	660	1.64	0.0024	0.0021	n.d.	0.0001	0.0004	0.0008	0.0019	n.d.	0.0020	0.0019
304	Oxybenzone	131-57-7	1176	1.73	0.0348	0.0267	0.0472	0.0290	0.0500	0.0168	0.0144	0.0196	0.0423	0.0483
305	Ethanone, 1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)-	68039-35-0	1038	1.13	n.d.	0.0281	n.d.	n.d.	0.2037	n.d.	n.d.	n.d.	n.d.	n.d.
Carboxylic acids														
306	Acetic acid	64-19-7	123	0.65	n.d.	1.3529	0.4526	1.1274	0.3727	n.d.	0.5299	n.d.	0.9898	0.4081
307	Propanoic acid	79-09-4	177	0.71	n.d.	n.d.	0.8625	0.6589	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
308	Butanoic acid	107-92-6	249	0.73	n.d.	n.d.	n.d.	0.1591	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
309	Hexanoic acid	142-62-1	417	0.85	n.d.	n.d.	n.d.	n.d.	1.1703	n.d.	4.4463	n.d.	n.d.	n.d.
310	Heptanoic acid	111-14-8	507	0.85	n.d.	0.4566	0.0559	0.2950	n.d.	0.7867	n.d.	0.2605	1.3939	1.5215
311	Octanoic acid	124-07-2	594	0.88	0.4862	0.8874	0.4506	0.6377	0.5176	0.3300	0.5796	0.2185	0.5531	0.4448
312	Nonanoic acid	112-05-0	675	0.90	n.d.	0.7561	0.4197	0.8261	0.4854	0.6852	1.0776	0.2770	0.7832	1.1765
313	n-Decanoic acid	334-48-5	753	0.90	0.1339	0.3343	0.2052	0.4255	0.3790	0.0578	0.1843	0.1078	0.8486	0.5783
314	Undecanoic acid	112-37-8	828	0.88	0.0233	n.d.	0.7589	0.2730	0.0548	0.0712	0.0824	0.6925	0.3210	0.1105
315	Dodecanoic acid	143-07-7	900	0.90	0.3676	0.3768	0.7563	0.4457	0.4953	0.2022	0.1937	0.2998	0.3016	0.3151
316	Tridecanoic acid	638-53-9	969	0.89	0.1573	0.1447	0.2264	0.1298	0.1556	0.0568	0.0564	0.0691	0.1391	0.1142
317	Tetradecanoic acid	544-63-8	1035	0.93	1.0189	1.1210	2.8500	1.1866	0.8575	0.5816	0.5931	0.7843	1.2504	1.6750

318	Pentadecanoic acid	1002-84-2	1098	0.91	0.8623	0.7361	1.8533	n.d.	1.0637	0.3805	0.3769	0.5627	0.7587	1.1440
319	n-Hexadecanoic acid	57-10-3	1155	0.93	4.2953	2.6852	3.4126	n.d.	4.3010	1.0806	1.1817	1.6106	1.9821	3.1824
320	Heptadecanoic acid	506-12-7	1212	0.91	n.d.	0.3387	n.d.	n.d.	n.d.	0.1555	0.0865	n.d.	n.d.	n.d.
321	Octadecanoic acid	57-11-4	1269	0.98	1.8148	n.d.	n.d.	n.d.	1.0606	0.8169	0.7320	0.4019	2.1451	2.8790
322	Nonadecanoic acid	646-30-0	1317	0.92	n.d.	n.d.	0.4783	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
323	Eicosanoic acid	506-30-9	1371	0.93	n.d.	0.3136	0.7181	n.d.	n.d.	0.1603	0.1718	0.2081	0.3661	0.3221
324	Hexanoic acid, 2-ethyl-	149-57-5	549	0.85	0.0768	0.5467	0.2633	0.5168	0.2491	0.7373	0.7671	0.6614	1.3472	2.0363
325	4-Methyloctanoic acid	54947-74-9	942	0.92	n.d.	n.d.	n.d.	n.d.	0.3951	n.d.	n.d.	n.d.	n.d.	n.d.
326	Z-7-Tetradecenoic acid	0-00-0	1020	0.95	n.d.	0.2918	1.0661	0.3498	0.4743	0.1282	0.0927	0.0956	0.2271	0.1905
327	Myristoleic acid	544-64-9	1020	0.95	0.3040	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
328	Hexadecenoic acid, Z-11-	2416-20-8	1143	0.98	n.d.	0.3806	n.d.	n.d.	n.d.	n.d.	0.3644	0.2165	0.3733	n.d.
329	Palmitoleic acid	373-49-9	1143	0.98	n.d.	0.8433	2.5115	1.1987	1.4845	0.2376	n.d.	0.5421	1.0581	1.0032
330	cis-10-Heptadecenoic acid	29743-97-3	1200	0.96	0.4968	n.d.	0.7644	n.d.	0.6227	n.d.	n.d.	n.d.	n.d.	n.d.
331	9,12-Octadecadienoic acid (Z,Z)-	60-33-3	1245	1.00	n.d.	n.d.	1.3771	n.d.	n.d.	0.4027	n.d.	0.5027	n.d.	n.d.
332	Oleic Acid	112-80-1	1254	0.95	n.d.	0.5129	1.1172	n.d.	1.5712	0.4731	0.5285	0.4816	0.2852	0.2834
333	cis-11-Eicosenoic acid	5561-99-9	1353	0.98	n.d.	n.d.	0.3972	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
334	L-Lactic acid	79-33-4	360	0.86	2.3877	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	2.6885	n.d.
335	Benzoic acid	65-85-0	591	1.10	0.2164	0.3235	n.d.	0.3787	n.d.	0.3271	0.4696	0.3165	n.d.	0.4053
336	Benzoic acid, p-tert-butyl-	98-73-7	852	1.09	n.d.	n.d.	0.0150	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
337	Oxalic acid	144-62-7	195	0.61	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2041	n.d.	n.d.
338	Methyltartronic acid	595-98-2	525	0.63	0.2285	n.d.	n.d.	0.0521	0.2166	0.5280	0.7629	0.3772	0.4193	0.5626
339	1,2-Benzenedicarboxylic acid	88-99-3	693	1.75	0.0064	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Esters														
340	Methyl formate	107-31-3	567	1.13	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0665	0.4953	n.d.
341	Propanoic acid, octyl ester	142-60-9	699	0.85	0.0757	0.5719	0.3414	0.2670	0.2590	n.d.	n.d.	n.d.	0.4542	n.d.
342	Pentanoic acid, octyl ester	5451-85-4	774	0.83	n.d.	0.2854	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
343	Dodecanoic acid, 1-methylethyl ester	10233-13-3	945	0.83	n.d.	n.d.	0.2233	0.6189	0.3171	0.1323	0.1046	0.1516	0.2740	0.1205
344	Hexadecanoic acid, methyl ester	112-39-0	1134	0.87	n.d.	n.d.	n.d.	n.d.	n.d.	0.1420	0.1497	0.1602	n.d.	n.d.
345	Isopropyl myristate	110-27-0	1074	0.83	0.7109	0.6799	0.5177	3.8086	1.7552	0.0764	0.1924	n.d.	n.d.	n.d.
346	Isopropyl palmitate	142-91-6	1191	0.84	0.5656	0.4749	0.5345	0.7299	0.7673	0.2088	0.1460	0.2792	0.3582	0.6364
347	1,2,3-Propanetriol, 1-acetate	106-61-6	522	1.28	0.0168	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

348	1-Methoxy-2-propyl acetate	108-65-6	291	0.91	n.d.	n.d.	0.0509	n.d.	0.3576	n.d.	n.d.	n.d.	n.d.	0.8716
349	Benzenemethanol, α-methyl-, acetate	93-92-5	594	1.17	n.d.	n.d.	n.d.	n.d.	0.0643	n.d.	n.d.	n.d.	n.d.	n.d.
350	Acetic acid, octyl ester	112-14-1	621	0.86	0.0264	0.2118	n.d.	0.1393	0.0956	n.d.	n.d.	n.d.	0.1090	0.0081
351	Benzeneethanol, α,α-dimethyl-, acetate	151-05-3	708	1.08	0.0084	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
352	4,7-methano-1H-inden-5-ol, 3a,4,5,6,7,7a-hexahydro-, acetate	0-00-0	789	1.17	0.0113	0.0067	0.0038	n.d.	0.0119	n.d.	n.d.	n.d.	0.0072	n.d.
353	Bornyl acetate	76-49-3	687	0.98	0.0279	n.d.	n.d.	n.d.	0.0339	n.d.	n.d.	n.d.	n.d.	n.d.
354	4-tert-Butylcyclohexyl acetate	32210-23-4	693	0.92	0.0415	0.0534	n.d.	0.2560	0.0454	n.d.	n.d.	0.1178	0.0634	n.d.
355	Nopyl acetate	128-51-8	795	0.99	0.0355	n.d.	0.0441	n.d.	0.0383	0.0184	n.d.	0.0635	0.0213	n.d.
356	1-Tetradecyl acetate	638-59-5	1182	0.86	n.d.	n.d.	n.d.	n.d.	n.d.	0.1476	n.d.	n.d.	n.d.	n.d.
357	1-Hexadecanol, acetate	629-70-9	1290	0.88	1.0681	0.4111	0.5469	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
358	Oxiraneoctanoic acid, 3-octyl-, methyl ester, trans-	6084-76-0	1329	1.05	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0411	n.d.	n.d.
359	1-Acetoxynonadecane	1577-43-1	1290	0.87	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2452	n.d.	n.d.	n.d.
360	2-Butoxyethyl acetate	112-07-2	504	0.97	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2165	n.d.
361	Acetic acid, phenylmethyl ester	140-11-4	567	1.25	n.d.	0.0510	0.0003	n.d.	0.0066	n.d.	0.0891	0.1846	0.0276	0.0540
362	2(5H)-Furanone	497-23-4	312	1.91	0.0059	0.0262	0.0068	0.0335	0.0239	0.0203	0.0479	0.0166	0.0576	0.0278
363	Butyrolactone	96-48-0	309	1.88	n.d.	n.d.	n.d.	n.d.	n.d.	0.0021	0.0163	n.d.	0.0346	0.0185
364	2(3H)-Furanone, dihydro-4-hydroxy-	5469-16-9	558	1.98	0.0270	0.0410	0.0486	0.0826	n.d.	0.0929	0.0901	0.0916	0.1727	0.1482
365	4-Methyl-5H-furan-2-one	6124-79-4	435	1.95	0.0012	0.0023	n.d.	0.0022	n.d.	0.0045	n.d.	0.0017	0.0026	0.0023
366	2H-Pyran-2-one, tetrahydro-	542-28-9	441	2.03	n.d.	0.0014	n.d.	0.0130	0.0058	n.d.	0.0072	n.d.	n.d.	0.0143
367	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	348	1.70	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0012	n.d.
368	(S)-(+)-2',3'-Dideoxyribonolactone	32780-06-6	579	2.00	0.0036	n.d.	n.d.	n.d.	0.0054	0.0091	0.0277	n.d.	n.d.	n.d.
369	2(3H)-Furanone, 5-ethyldihydro-	695-06-7	447	1.63	n.d.	0.0162	n.d.	n.d.	n.d.	0.0072	0.0180	0.0077	0.0118	0.0108
370	2(3H)-Furanone, 5-acetyldihydro-	29393-32-6	501	2.20	0.0014	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0007
371	2(3H)-Furanone, dihydro-5-propyl-	105-21-5	543	1.52	0.0026	0.0043	n.d.	0.0057	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
372	2(3H)-Furanone, 5-butyldihydro-	104-50-7	636	1.45	0.0078	0.0048	n.d.	0.0062	0.0073	n.d.	0.0027	0.0060	0.0113	n.d.
373	2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	726	1.37	0.0103	n.d.	0.0085	0.0139	0.0131	0.0100	n.d.	0.0114	0.0237	0.0169
374	2(3H)-Furanone, 5-hexyldihydro-	706-14-9	810	1.32	0.0066	0.0045	0.0109	0.0062	0.0074	n.d.	0.0033	0.0064	0.0131	0.0100
375	2(3H)-Furanone, 5-heptyldihydro-	104-67-6	888	1.28	0.0327	0.0061	0.0164	0.0131	0.0131	0.0121	0.0148	0.0318	0.0165	0.0171

376	2(3H)-Furanone, 5-dodecyldihydro-	730-46-1	1221	1.19	0.0041	n.d.	n.d.	n.d.	n.d.	0.0022	0.0172	n.d.	n.d.	n.d.
377	Ethylene brassylate	105-95-3	1176	1.37	0.0109	0.0092	n.d.	0.0432	0.0105	n.d.	0.0088	n.d.	0.0090	0.0036
378	Oxacyclotetradecane-2,11-dione, 13-methyl-	74685-36-2	1077	1.15	0.0550	0.1084	0.8837	n.d.	0.0303	0.1288	0.2094	n.d.	0.1213	0.2504
379	1,4-Dioxacyclohexadecane-5,16-dione	54982-83-1	1116	1.40	0.0139	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
380	Dehydromevalonic lactone	2381-87-5	546	1.94	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0012	n.d.
381	1(3H)-Isobenzofuranone	87-41-2	708	1.98	0.0031	0.0030	0.0010	0.0008	0.0014	n.d.	n.d.	n.d.	0.0009	0.0008
382	Coumarin	91-64-5	783	1.92	n.d.	n.d.	n.d.	0.0055	n.d.	0.0024	n.d.	0.0050	0.0028	0.0053
383	1,6-Dioxacyclododecane-7,12-dione	777-95-7	864	1.65	n.d.	n.d.	n.d.	0.0057	n.d.	n.d.	0.0083	0.0059	0.0173	n.d.
384	Propanoic acid, 2-hydroxy-, methyl ester, (ñ)-	2155-30-8	96	0.80	n.d.	n.d.	n.d.	0.6060	n.d.	n.d.	n.d.	n.d.	n.d.	0.3066
385	Propanoic acid, 2-hydroxy-, ethyl ester	97-64-3	603	0.58	n.d.	0.4355	n.d.	0.1429	n.d.	0.0566	n.d.	0.0583	0.5265	0.1571
386	Propanoic acid, 2-methyl-, 3-hydroxy-2,2,4-trimethylpentyl ester	77-68-9	756	0.97	n.d.	0.3938	n.d.	0.2137	0.8511	0.0199	0.4132	n.d.	n.d.	0.0599
387	Pentanoic acid, 2,2,4-trimethyl-3-hydroxy-, isobutyl ester	244074-78-0	741	1.03	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.6591	n.d.	n.d.	n.d.
388	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	23470-00-0	1428	1.17	n.d.	n.d.	0.0503	n.d.	0.0100	n.d.	n.d.	n.d.	n.d.	n.d.
389	Benzoic acid, methyl ester	93-58-3	507	1.21	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0013	n.d.	n.d.	n.d.
390	Benzyl Benzoate	120-51-4	1020	1.54	0.0110	0.0938	0.0075	0.0161	0.0169	0.0372	0.0197	0.0080	0.0192	0.1492
391	Benzoic acid, 2-benzoyl-, methyl ester	606-28-0	1116	1.90	0.0049	n.d.	n.d.	0.0060	n.d.	n.d.	0.0056	n.d.	n.d.	0.0042
392	1,2-Ethanediol, dibenzoate	94-49-5	1419	1.53	0.0009	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0013
393	Benzoic acid, tridecyl ester	0-00-0	1335	1.08	0.0975	0.1762	0.3586	0.2285	0.1923	0.0672	0.0896	0.1133	0.1782	0.1227
394	Benzoic acid, tetradecyl ester	0-00-0	1386	1.08	0.1783	0.1073	n.d.	0.1194	n.d.	n.d.	0.0518	0.0656	0.1048	0.0776
395	Benzoic acid, pentadecyl ester	0-00-0	1434	1.10	0.0512	n.d.	0.4827	0.2245	0.0921	0.0278	0.0265	0.0391	0.0566	0.0463
396	Dimethyl phthalate	131-11-3	798	1.57	0.0003	n.d.	n.d.	0.0006	0.0008	n.d.	0.0007	n.d.	0.0019	0.0018
397	Diethyl Phthalate	84-66-2	903	1.44	0.0251	0.0166	0.0351	0.1588	0.0248	0.0078	0.0104	0.0152	0.0945	0.0453
398	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	1083	1.26	0.0790	0.1082	0.1353	0.1904	0.0843	0.0625	0.0928	0.0580	0.1397	0.0952
399	Dibutyl phthalate	84-74-2	1140	1.31	0.1805	0.1068	0.1224	0.1436	0.2148	0.1640	0.1403	0.1027	0.1799	0.1121
400	Benzyl butyl phthalate	85-68-7	1341	1.69	n.d.	n.d.	n.d.	n.d.	n.d.	0.0104	n.d.	n.d.	n.d.	0.0187

401	Diisooctyl phthalate	131-20-4	1446	1.18	0.4528	0.4536	n.d.	n.d.	n.d.	0.3611	0.3024	n.d.	n.d.	0.4058
402	Phthalic acid, bis(7-methyloctyl) ester	20548-62-3	1548	1.35	n.d.	n.d.	n.d.	n.d.	n.d.	0.0093	n.d.	n.d.	n.d.	0.0102
403	1,2-Benzenedicarboxylic acid, bis(8-methylnonyl) ester	89-16-7	1575	1.34	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0082	n.d.
404	Methyl salicylate	119-36-8	600	1.20	0.0263	0.0475	0.0619	0.0531	0.0637	0.0415	0.0877	0.0806	n.d.	n.d.
405	Benzoic acid, 2-hydroxy-, pentyl ester	2050-08-0	903	1.09	n.d.	n.d.	n.d.	n.d.	0.0168	0.0033	n.d.	n.d.	n.d.	0.0211
406	cis-3-Hexenyl salicylate	65405-77-8	966	1.14	0.0085	n.d.	n.d.	0.1151	0.0121	n.d.	0.0033	n.d.	n.d.	n.d.
407	n-Hexyl salicylate	6259-76-3	972	1.08	0.0649	0.1041	0.1534	n.d.	0.0899	n.d.	0.0415	n.d.	n.d.	0.0615
408	Benzoic acid, 2-hydroxy-, phenylmethyl ester	118-58-1	1086	1.50	0.0623	0.1541	0.0923	0.2460	0.1038	0.0238	0.0361	0.0440	0.0546	0.0407
409	Phenylethyl salicylate	87-22-9	1140	1.50	n.d.	0.0045	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
410	2-Ethylhexyl salicylate	118-60-5	1059	1.05	n.d.	1.5151	2.1337	0.6910	0.8956	0.1777	0.3187	0.2917	0.4058	0.4218
411	Homosalate	118-56-9	1092	1.13	0.1017	0.4636	0.7913	1.6258	0.7740	0.1478	0.2892	0.2943	0.7119	0.5610
412	Methylparaben	99-76-3	816	1.41	n.d.	n.d.	0.0941	0.0104	n.d.	n.d.	n.d.	0.0073	n.d.	n.d.
413	Propylparaben	94-13-3	930	1.39	n.d.	n.d.	0.0634	n.d.	n.d.	n.d.	n.d.	n.d.	0.0069	n.d.
414	2-Propenoic acid, octyl ester	2499-59-4	651	0.88	n.d.	0.0115	0.0056	n.d.	0.3022	0.1454	n.d.	n.d.	n.d.	n.d.
415	Butanoic acid, 1,1-dimethyl-2-phenylethyl ester	10094-34-5	843	1.04	0.0379	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
416	Dodecyl acrylate	2156-97-0	987	0.87	0.1093	0.1336	0.1857	0.2185	0.2239	0.0488	0.1304	0.2073	0.2413	0.1466
417	n-Dodecyl methacrylate	142-90-5	1374	0.89	0.5705	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
418	cis-9-Tetradecenoic acid, heptyl ester	0-00-0	1641	1.29	0.1366	0.1966	0.4316	0.2656	0.3279	0.1350	0.0842	0.0624	0.1157	0.1259
419	cis-10-Pentadecenoic acid, heptyl ester	0-00-0	1704	1.48	n.d.	0.1956	0.2181	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0868
420	1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	137-89-3	1539	1.14	0.3032	0.2116	0.5837	0.3235	0.3921	n.d.	0.3839	0.4954	0.6600	0.6331
421	1,4-Dioxane-2,6-dione	4480-83-5	231	0.47	n.d.	n.d.	n.d.	0.0747	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
422	Acetic anhydride	108-24-7	813	0.96	n.d.	n.d.	0.7615	0.2343	n.d.	0.4474	n.d.	0.3336	0.4004	n.d.
423	Propylene Carbonate	108-32-7	372	2.07	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0127	n.d.	n.d.	n.d.
424	1,4-Dioxane-2,5-dione, 3,6-dimethyl-	95-96-5	537	2.06	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0047	n.d.	n.d.	n.d.
425	Oxiranecarboxylic acid, 3-methyl-3-phenyl-, ethyl ester, cis-	19464-95-0	861	1.29	0.0198	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

426	2-Phenoxyethyl isobutyrate	103-60-6	852	1.22	0.0144	n.d.	n.d.	0.0567	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
427	Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	24851-98-7	966	1.22	0.0936	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
428	Oxalic acid, allyl nonyl ester	0-00-0	1005	0.71	n.d.	0.4566	0.6278	0.5513	0.5282	n.d.	n.d.	0.7017	0.5953	n.d.
429	Oxalic acid, isobutyl nonyl ester	0-00-0	1581	0.91	n.d.	n.d.	n.d.	0.2366	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
430	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	924	0.90	n.d.	0.3556	0.0003	0.4340	0.2865	0.0499	0.6093	n.d.	n.d.	n.d.
431	Oxalic acid, allyl dodecyl ester	0-00-0	1128	0.75	n.d.	0.5216	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
432	1-Propene-1,2,3-tricarboxylic acid, tributyl ester	7568-58-3	1254	1.10	n.d.	0.0227	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
433	Oxalic acid, allyl tridecyl ester	0-00-0	1002	0.76	n.d.	n.d.	1.1144	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
434	Tributyl acetylcitrate	77-90-7	1305	1.13	0.1673	0.2009	0.3675	0.2633	0.1516	0.0938	0.0824	0.0865	0.2588	0.1589
435	Oxalic acid, allyl hexadecyl ester	0-00-0	789	0.68	n.d.	0.7472	n.d.	1.0220	n.d.	n.d.	0.5005	0.8817	0.3010	n.d.
436	Hexanedioic acid, bis(2-ethylhexyl) ester	103-23-1	1380	0.97	0.1121	0.0660	0.1703	0.1462	0.1041	0.0782	0.0436	0.0928	0.0956	0.0876
437	Oxalic acid, allyl octadecyl ester	0-00-0	1296	0.79	n.d.	1.5889	n.d.	n.d.	n.d.	n.d.	n.d.	0.3435	n.d.	n.d.
438	Carbonic acid, eicosyl vinyl ester	0-00-0	1443	0.81	n.d.	n.d.	1.9584	n.d.	1.3026	n.d.	n.d.	n.d.	0.9964	n.d.
439	Glycerol tricaprylate	538-23-8	1632	1.42	n.d.	n.d.	n.d.	0.6347	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
Nitrogen containing volatiles														
440	Hydrogen azide	7782-79-8	207	1.03	0.3735	n.d.	n.d.	0.0950	n.d.	n.d.	n.d.	0.2855	n.d.	n.d.
441	Nitrous oxide	10024-97-2	93	0.49	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1249	n.d.	0.0037	0.1604
442	Acetonitrile	75-05-8	102	0.56	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	1.6198	n.d.
443	Methyl isocyanide	593-75-9	219	0.53	n.d.	n.d.	n.d.	n.d.	n.d.	0.1933	0.0342	n.d.	n.d.	n.d.
444	Ethylenimine	151-56-4	105	2.10	n.d.	n.d.	0.0543	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0216
445	Acetamide	60-35-5	231	1.14	0.0888	0.0457	n.d.	0.1388	0.1213	0.1175	0.1110	0.0896	0.1732	0.0209
446	Ethanol, 2-nitro-	625-48-9	90	0.14	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.8101
447	Dimethylamine	124-40-3	354	0.67	n.d.	n.d.	n.d.	0.5173	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
448	1-Tetrazol-2-ylethanone	51410-11-8	126	0.62	n.d.	n.d.	n.d.	0.6439	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
449	Formamide, N,N-dimethyl-	68-12-2	222	1.19	n.d.	0.0541	0.0371	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0340
450	Propane, 2-nitro-	79-46-9	108	0.70	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2387	n.d.	n.d.	n.d.
451	dl-Alanine	302-72-7	396	0.26	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0613	n.d.

452	Alanine	56-41-7	720	0.43	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.4248
453	Methylamine, N,N-dimethyl-	75-50-3	102	2.20	0.0092	n.d.	n.d.	0.0241	n.d.	0.0239	0.0140	0.0138	n.d.	0.1007
454	(R)-(-)-2-Amino-1-propanol	35320-23-1	327	0.44	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0284	n.d.
455	Ethanamine, N-ethyl-	109-89-7	360	0.73	0.0153	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
456	1H-Pyrrole-2,5-dione	541-59-3	396	1.59	0.0116	0.0170	n.d.	0.0025	0.0084	n.d.	0.0251	n.d.	n.d.	n.d.
457	Pyrimidine-2,4(1H,3H)-dione, 5-amino-6-nitroso-	0-00-0	444	0.77	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.3315	n.d.
458	Pyrrole	109-97-7	195	0.93	n.d.	0.3468	0.1058	n.d.	n.d.	0.4330	0.3209	n.d.	0.6115	0.3597
459	Succinimide	123-56-8	528	1.98	0.0087	0.0112	0.0045	0.0277	0.0182	0.0280	0.0428	0.0031	0.0382	0.0933
460	3(2H)-Isothiazolone, 2-methyl-	2682-20-4	567	2.06	0.0074	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
461	2,4-Imidazolidinedione, 5-methyl-	616-03-5	759	1.53	n.d.	n.d.	n.d.	n.d.	n.d.	0.0480	0.0849	n.d.	n.d.	0.1620
462	2,5-Piperazinedione	106-57-0	918	2.53	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0603
463	Aziridine, 1-ethenyl-	5628-99-9	147	0.83	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.8209	3.3521	1.7146
464	2-Pyrrolidinone	616-45-5	489	1.70	0.0068	0.0043	0.0034	0.0147	0.0090	0.0174	0.0137	0.0186	0.0495	0.0514
465	N-Glycylglycine	556-50-3	909	2.62	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0385	n.d.	n.d.	n.d.
466	Allantoic acid	99-16-1	345	0.44	n.d.	n.d.	n.d.	0.2423	n.d.	0.0481	n.d.	n.d.	n.d.	n.d.
467	Cyclobutylamine	2516-34-9	261	0.52	0.2108	0.3716	0.1197	0.7394	n.d.	0.8560	0.4676	0.0059	0.1999	0.0633
468	Formamide, N,N-diethyl-	617-84-5	345	1.27	0.0643	0.0368	0.0514	0.1216	0.0993	n.d.	n.d.	n.d.	n.d.	0.0683
469	Ornithine	70-26-8	771	1.37	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2196
470	4-Vinyl-imidazole	3718-04-5	657	1.19	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.2821	0.3150	1.0388	1.5023
471	1H-Pyrrole, 2-methyl-	636-41-9	270	1.02	0.0595	n.d.	n.d.	n.d.	n.d.	n.d.	0.1840	n.d.	n.d.	n.d.
472	l-Pyrrolid-2-one, N-carbamoyl-	40451-67-0	957	2.39	n.d.	n.d.	n.d.	n.d.	n.d.	0.2785	0.4593	n.d.	0.4743	1.8623
473	2-Piperidinone	675-20-7	585	1.75	0.0040	0.0121	n.d.	0.0165	n.d.	0.0128	0.0171	0.0288	n.d.	0.0194
474	2-Pyrrolidinone, 1-methyl-	872-50-4	450	1.62	n.d.	n.d.	n.d.	0.0093	n.d.	0.0078	0.0100	0.0070	0.0104	0.0094
475	N-Formylmorpholine	4394-85-8	513	1.94	n.d.	n.d.	n.d.	0.0007	n.d.	n.d.	n.d.	n.d.	n.d.	0.0004
476	3,6-Dimethylpiperazine-2,5-dione	5625-46-7	852	2.21	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0058	n.d.	n.d.	0.0045
477	5-Isopropyl-2,4-imidazolidinedione	16935-34-5	795	1.80	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0033	0.0132
478	Caprolactam	105-60-2	642	1.75	n.d.	n.d.	n.d.	0.0061	0.0028	n.d.	n.d.	n.d.	n.d.	n.d.
479	n-Butylethylenediamine	19522-69-1	483	0.73	n.d.	0.3383	n.d.	0.9583	n.d.	n.d.	0.5671	n.d.	n.d.	n.d.
480	Ethanone, 1-(1H-pyrrol-2-yl)-	1072-83-9	471	1.41	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1102	n.d.

481	1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-	5768-79-6	801	2.04	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0059	n.d.	0.0076	0.0098
482	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-	19179-12-5	984	2.99	n.d.	0.0099	n.d.	n.d.	0.0166	n.d.	0.0127	n.d.	0.0097	0.0057
483	2,4-Imidazolidinedione, 5-(2-methylpropyl)-, (S)-	40856-75-5	876	1.67	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0601	n.d.	n.d.	n.d.
484	Benzothiazole	95-16-9	618	1.58	0.0307	n.d.	n.d.	0.0169	n.d.	n.d.	n.d.	0.0041	n.d.	0.0258
485	Salicyl hydrazide	936-02-7	813	1.44	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0119
486	1,7-Dimethylxanthine	611-59-6	1101	2.13	n.d.	n.d.	n.d.	n.d.	n.d.	0.0049	0.0117	n.d.	n.d.	0.0439
487	Theobromine	83-67-0	1071	2.39	n.d.	n.d.	n.d.	n.d.	n.d.	0.0094	0.0113	n.d.	0.0506	0.0603
488	4-Cyanocyclohexene	100-45-8	417	1.45	n.d.	n.d.	n.d.	n.d.	0.0015	n.d.	n.d.	n.d.	n.d.	n.d.
489	Caffeine	58-08-2	1056	2.20	0.0188	0.0307	0.0517	0.0198	0.0396	0.0925	0.0926	0.0928	0.1908	0.2282
490	Pyridine, 2,4,6-trimethyl-	108-75-8	420	1.05	n.d.	n.d.	n.d.	n.d.	0.1765	n.d.	n.d.	n.d.	n.d.	n.d.
491	1-Butanamine, N-butyl-N-nitroso-	924-16-3	657	1.09	0.0249	n.d.	0.0084	0.0346	0.0053	n.d.	n.d.	0.0911	n.d.	0.0848
492	o-Cyanobenzoic acid	3839-22-3	807	1.86	n.d.	n.d.	n.d.	n.d.	n.d.	0.0033	n.d.	n.d.	n.d.	n.d.
493	Benzyl nitrile	140-29-4	528	1.64	0.0023	0.0035	0.0021	0.0068	0.0032	0.0151	0.0088	0.0015	0.0074	0.0500
494	Indole	120-72-9	675	1.64	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0127	n.d.	n.d.	0.0025
495	5H-1-Pyrindine	270-91-7	675	1.64	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0110	n.d.
496	5H-1-Pyrindine, 6,7-dihydro-	533-37-9	522	1.34	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0642	0.0245
497	Benzene, (1-nitroethyl)-	7214-61-1	666	1.54	0.0214	n.d.	0.0031	0.0117	0.0091	n.d.	n.d.	n.d.	n.d.	n.d.
498	Oxime-, methoxy-phenyl-_	0-00-0	348	0.76	n.d.	0.1268	n.d.	0.0960	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
499	Phenol, 4-[2-(methylamino)ethyl]-	370-98-9	285	0.36	n.d.	n.d.	0.0025	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
500	2-Benzyloxyethylamine	38336-04-8	735	1.30	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0076	0.0046
501	dl-Alanyl-l-leucine	1638-60-4	990	1.87	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0143
502	Formamide, N,N-dibutyl-	761-65-9	690	1.10	0.0515	0.0307	0.0161	0.1013	0.0745	0.0967	0.0444	0.0567	0.1209	0.3134
503	Benzonitrile, 3,5-dimethyl-	22445-42-7	585	1.32	0.0204	0.0240	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
504	3-(4-Hydroxyphenyl) propionitrile	17362-17-3	879	1.88	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0015	n.d.	n.d.	n.d.
505	Methane, nitroso-	865-40-7	96	0.74	n.d.	0.2806	0.3636	n.d.	n.d.	n.d.	1.7587	1.0856	1.0170	0.7544
506	Formamide	75-12-7	453	0.72	n.d.	n.d.	n.d.	n.d.	n.d.	1.1025	0.9539	0.1619	n.d.	n.d.
507	Urea	57-13-6	459	0.43	n.d.	0.1911	0.1029	0.2955	0.1825	2.5474	3.3424	3.2125	7.6833	5.1956
508	N,N-Dimethyloctylamine	7378-99-6	870	0.75	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1158	n.d.	n.d.	n.d.

509	1H-Indole, 1,2,3-trimethyl-	1971-46-6	864	1.46	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0023	n.d.	n.d.	n.d.
510	Parbenate	10287-53-3	984	1.50	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0006	n.d.	n.d.	n.d.
511	2-Pyrrolidinone, 5-(cyclohexylmethyl)-	14293-08-4	1398	1.40	n.d.	0.0016	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0033	n.d.
512	5(4H)-Oxazolone, 2-methyl-4-(phenylmethylene)-	881-90-3	888	2.17	n.d.	0.0025	n.d.	n.d.	0.0038	n.d.	0.0038	n.d.	0.0006	n.d.
513	2,5-Piperazinedione, 3-methyl-6-(phenylmethyl)-	14474-78-3	1206	2.53	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0054	n.d.	0.0156	n.d.
514	Diethyltoluamide	134-62-3	897	1.38	0.0074	0.0107	0.0091	0.0094	0.0068	0.0192	0.0208	0.0246	0.0601	0.0266
515	Dodecanamide	1120-16-7	1263	1.18	n.d.	n.d.	0.1833	n.d.	n.d.	0.0898	0.1113	0.0159	0.0639	0.1685
516	Drometrizole	2440-22-4	1203	1.60	0.0025	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
517	Dibenzylamine	103-49-1	996	1.43	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0015	n.d.
518	2-Propenenitrile, 3,3-diphenyl-	3531-24-6	1080	1.79	0.0058	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
519	Etocrylene	5232-99-5	1251	1.79	0.0086	0.0285	0.0604	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
520	9-Octadecenamide, (Z)-	301-02-0	1353	1.25	n.d.	0.0019	0.0096	0.0080	n.d.	n.d.	0.0006	n.d.	0.0051	0.0041
521	Octocrylene	6197-30-4	1494	1.59	0.2759	0.3635	0.6368	0.4228	0.3172	0.1194	0.1188	0.1926	0.2990	0.2961
522	Cholesta-4,6-dien-3-ol, (3β)-	14214-69-8	1608	1.59	0.0059	0.0111	n.d.	n.d.	n.d.	0.0060	n.d.	n.d.	n.d.	0.0003
Halogen containing volatiles														
523	Benzyl chloride	100-44-7	429	1.17	0.0721	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0324	n.d.
524	Benzene, 1,3-dichloro-	541-73-1	429	1.14	0.0078	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
525	Chloroxylenol	88-04-0	759	1.27	n.d.	0.0012	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
526	Cyclopropanecarboxylic acid, 3-(2,2-dichlorovinyl)-2,2-dimethyl-, (3-phenoxyphenyl) methyl ester, (1R-trans)-	51877-74-8	1512	1.70	n.d.	n.d.	n.d.	n.d.	0.0093	n.d.	n.d.	n.d.	n.d.	n.d.
527	Cholest-5-en-3-ol (3β)-, carbonochloridate	7144-08-3	1620	1.62	n.d.	n.d.	0.0013	0.0029	0.0381	n.d.	n.d.	0.0071	0.0024	0.0005
528	Ethyne, fluoro-	2713-09-9	90	2.53	n.d.	n.d.	0.0047	n.d.	n.d.	n.d.	n.d.	0.0310	n.d.	n.d.
529	1-Fluorooctane	463-11-6	594	0.85	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.4997	n.d.	n.d.	n.d.
530	1-Iodo-2-methylundecane	73105-67-6	1188	0.80	0.0625	0.8146	n.d.	0.0815	0.4718	0.0454	0.8591	0.6679	0.5399	0.7434
531	Tetradecane, 1-iodo-	19218-94-1	936	0.74	0.0445	0.1071	1.5890	n.d.	0.1602	0.0131	0.9321	0.5009	1.0204	0.1154

Sulphur containing volatiles														
532	Carbonyl sulfide	463-58-1	546	0.42	n.d.	0.0434	n.d.	n.d.	0.6060	n.d.	n.d.	n.d.	n.d.	n.d.
533	Carbon disulfide	75-15-0	90	2.15	n.d.	0.2064	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0158
534	Sulfur dioxide	7446-09-5	354	0.45	0.0028	0.1977	0.0671	n.d.	n.d.	0.0570	0.1796	0.0703	0.1782	0.7431
535	Methanethiol	74-93-1	504	0.44	n.d.	n.d.	n.d.	n.d.	n.d.	0.0499	n.d.	n.d.	n.d.	n.d.
536	Diphenyl sulfone	127-63-9	1104	2.19	0.0064	0.0082	0.0129	0.0100	n.d.	0.0080	0.0117	0.0055	0.0201	0.0167
537	2-Undecanethiol, 2-methyl-	10059-13-9	816	0.71	0.9423	1.0537	0.1430	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
538	Dimethyl sulfone	67-71-0	309	2.24	0.3333	0.9597	0.5622	0.5679	0.2250	0.7313	0.7201	1.1236	1.5857	1.1718
539	Dimethyl Sulfoxide	67-68-5	273	1.50	0.0121	0.0262	0.0295	0.1789	0.0446	0.0106	0.0139	0.0338	0.0483	0.1048
Other compounds														
540	Carbon dioxide	124-38-9	93	0.01	n.d.	n.d.	0.0026	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
541	Boronic acid, ethyl-	4433-63-0	396	0.90	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.9468	n.d.	n.d.	n.d.
542	Ethylamine, 2-((p-bromo-α-methyl-α-phenylbenzyl) oxy)-N,N-dimethyl-	3565-72-8	1242	0.79	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1559	n.d.	n.d.	n.d.
543	N-Dimethylaminomethyl-tert-butyl-isopropylphosphine	83718-54-1	1299	1.09	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.1455	n.d.	n.d.
544	Ethanol, 2-butoxy-, phosphate (3:1)	78-51-3	1377	1.20	n.d.	n.d.	n.d.	n.d.	n.d.	0.0068	0.0040	n.d.	0.0037	0.0101
545	Benzyl 2-chloroethyl sulfone	66998-67-2	1116	2.26	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.0263	n.d.

a) First dimension retention time
b) Second dimension retention time
c) Peak areas were normalised using the TIC of the eucalyptol IS
d) Ankle observations n=2 (not 3) due to power outages
e) Not detected

Table S2. Compounds detected and tentatively identified during the analysis of the human skin surface originating from the ankle and wrist area using an in-house developed PDMS sampler with inlet TD-GC×GC-TOFMS. The compounds listed here are limited to those that were previously reported in literature to elicit a response in mosquitoes.

#	Compound	CAS Number	1D RT[c] (s)	2D RT[d] (s)	1D RI_{exp}	1D RI_{Lit} NIST14	Response reported in mosquitoes	Wrist (m=15)[a] Count (n=5)[e]	Mean[f]	Median	Range		Ankles (m=14)[a,b] Count (n=5)[e]	Mean	Median	Range	
											Min	Max				Min	Max
Benzyl and phenyl hydrocarbons																	
1	Benzene, 1-methyl-3-propyl-	1074-43-7	477	0.87	1042	1042	[63]	3	0.0425	0.0501	0.0031	0.0742	2	0.3399	0.3399	0.1602	0.5196
Alkenes																	
2	Tridecane	629-50-5	711	0.69	1305	1300	[63]	3	0.2269	0.1945	0.1331	0.3532	4	0.2416	0.2212	0.0906	0.4336
Alcohols																	
3	Phenol	108-95-2	405	1.11	966	957	[51]	2	0.0329	0.0329	0.0324	0.0335	4	0.4255	0.4530	0.0358	0.7603
4	Phenol, 2-methyl-	95-48-7	496	1.13	1039	1062	[10, 51]	1	0.0733	0.0733	0.0733	0.0733	0	n.d.[g]	n.d.	n.d.	n.d.
5	Phenylethyl Alcohol	60-12-8	522	1.30	1090	1088	[36, 40, 41, 61, 64, 65]	5	0.0268	0.0298	0.0128	0.0420	5	0.0226	0.0160	0.0115	0.0448
6	Ethanol, 2-phenoxy-	122-99-6	615	1.43	1190	1193	[51]	5	0.1834	0.1031	0.0810	0.4885	1	0.0207	0.0207	0.0207	0.0207
7	Dihydromyrcenol	18479-58-8	498	0.83	1065	1062	[46]	2	0.0876	0.0876	0.0682	0.1070	1	0.2588	0.2588	0.2588	0.2588
8	1-Dodecanol	112-53-8	834	0.88	1463	1462	[36, 66]	3	0.5133	0.5303	0.2785	0.7313	4	0.3057	0.3672	0.0098	0.4785
Aldehydes																	
9	Benzaldehyde	100-52-7	372	1.28	931	933	[46, 61, 67]	0	n.d.	n.d.	n.d.	n.d.	1	0.0162	0.0162	0.0162	0.0162
10	Benzeneacetaldehyde	122-78-1	450	1.36	1013	1011	[57]	2	0.0287	0.0287	0.0144	0.0430	4	0.0586	0.0693	0.0044	0.0913
11	Octanal	124-13-0	423	0.90	984	982	[41, 45, 46, 61, 62]	4	0.9506	0.9288	0.7263	1.2186	5	1.1213	1.2850	0.4831	1.7305
12	2-Nonenal, (*E*)-	18829-56-6	567	0.98	1139	1135	[57]	5	0.0559	0.0522	0.0189	0.0873	5	0.0921	0.0841	0.0212	0.2029
13	Nonanal	124-19-6	519	0.92	1087	1083	[47, 61]	5	0.6161	0.6136	0.3415	1.0918	5	0.9046	1.0846	0.2414	1.4267
14	2,6-Octadienal, 3,7-dimethyl-, (*E*)-	141-27-5	663	1.07	1247	1249	[57]	5	0.0110	0.0097	0.0025	0.0224	5	0.0274	0.0271	0.0146	0.0383

15	Decanal	112-31-2	612	0.91	1187	1185	[46, 47, 61, 63]	3	0.1621	0.1500	0.1025	0.2337	5	0.2616	0.3491	0.0198	0.4590
16	Undecanal	112-44-7	699	0.90	1291	1287	[20]	4	0.0768	0.0649	0.0571	0.1201	2	0.1314	0.1314	0.1266	0.1362
17	Dodecanal	112-54-9	780	0.89	1389	1389	[48]	3	0.0657	0.0363	0.0342	0.1265	1	0.0427	0.0427	0.0427	0.0427
Ketones																	
18	Cyclohexanone	108-94-1	309	1.16	866	871	[67]	0	n.d.	n.d.	n.d.	n.d.	1	0.0447	0.0447	0.0447	0.0447
19	Acetophenone	98-86-2	474	1.35	1039	1042	[47, 61]	3	0.0720	0.0169	0.0007	0.1985	3	0.0882	0.0977	0.0637	0.1031
20	5-Hepten-2-one, 6-methyl-	110-93-0	405	0.97	966	964	[36, 46, 47, 50, 54, 66]	4	0.4340	0.2962	0.1098	1.0335	4	0.3990	0.4709	0.0076	0.6467
21	2-Octanone	111-13-7	414	0.88	975	971	[61]	5	1.1737	0.8767	0.0330	3.0408	3	0.6431	0.8546	0.1978	0.8770
22	5,9-Undecadien-2-one, 6,10-dimethyl-, (*E*)-	3796-70-1	813	0.98	1433	1429	[46, 50, 54, 66]	1	0.1337	0.1337	0.1337	0.1337	3	0.1277	0.1638	0.0316	0.1876
23	2-Tridecanone	593-08-8	849	0.89	1483	1477	[53]	5	0.0784	0.0696	0.0288	0.1313	5	0.0266	0.0209	0.0089	0.0628
Carboxylic acids																	
24	Hexanoic acid	142-62-1	417	0.85	978	982	[42, 44, 49, 50]	2	0.1588	0.1588	0.0461	0.2715	0	n.d.	n.d.	n.d.	n.d.
25	Heptanoic acid	111-14-8	507	0.85	1074	1078	[42, 44, 47, 49, 50, 68, 69]	2	0.0861	0.0861	0.0062	0.1661	1	0.7263	0.7263	0.7263	0.7263
26	Octanoic acid	124-07-2	594	0.88	1168	1173	[42, 44, 47, 49, 68, 69]	5	0.2865	0.4298	0.0240	0.4693	5	0.1852	0.1785	0.0327	0.3819
27	Nonanoic acid	112-05-0	675	0.90	1262	1272	[44, 49, 50]	5	0.3309	0.4225	0.0245	0.6627	2	0.1605	0.1605	0.0356	0.2855
28	*n*-Decanoic acid	334-48-5	753	0.90	1356	1362	[44, 49, 50]	4	0.1817	0.1573	0.0107	0.4016	2	0.5093	0.5093	0.1988	0.8198
29	Undecanoic acid	112-37-8	828	0.88	1454	1472	[44, 49]	2	0.0733	0.0733	0.0561	0.0905	1	0.0089	0.0089	0.0089	0.0089
30	Dodecanoic acid	143-07-7	900	0.90	1554	1556	[44, 47, 49, 50]	5	0.1734	0.1165	0.0423	0.3348	5	0.1390	0.1018	0.0902	0.2880
31	Tridecanoic acid	638-53-9	969	0.89	1655	1660	[44, 47, 49]	5	0.0567	0.0543	0.0155	0.1146	3	0.0365	0.0278	0.0216	0.0600
32	Tetradecanoic acid	544-63-8	1035	0.93	1755	1752	[19, 36, 41, 42, 44, 47, 49, 51, 68-71]	5	1.1887	1.0134	0.8761	1.9806	5	0.6524	0.4568	0.0840	1.3382
33	Palmitoleic acid	373-49-9	1143	0.98	1930	1936	[52]	5	1.8962	1.6416	0.8933	3.3539	4	0.7943	0.8244	0.2602	1.2682
34	*n*-Hexadecanoic acid	57-10-3	1155	0.93	1950	1954	[47]	4	2.2424	2.4197	0.4932	3.6370	4	1.8202	1.6843	0.6828	3.2294

35	Oleic Acid	112-80-1	1254	0.95	2128	2134	[52]	4	0.6208	0.6449	0.0707	1.1228	3	0.3619	0.3303	0.3196	0.4358
Esters																	
36	Methyl salicylate	119-36-8	600	1.20	1174	1174	[56, 72]	5	0.0210	0.0193	0.0052	0.0406	3	0.0414	0.0276	0.0154	0.0812
37	Hexadecanoic acid, methyl ester	112-39-0	1134	0.87	1915	1909	[52]	4	0.3005	0.2655	0.0977	0.5733	5	0.1687	0.1468	0.1111	0.2481
Terpenes																	
38	Limonene	138-86-3	462	0.79	1026	1017	[41]	2	0.0371	0.0227	0.0122	0.0764	1	0.4089	0.4089	0.4089	0.4089
39	Linalool	78-70-6	522	0.88	1090	1086	[36]	4	0.5598	0.5250	0.5598	0.6754	2	0.5508	0.5508	0.5317	0.5700
40	Citronellol	106-22-9	636	0.93	1215	1211	[57]	5	0.0635	0.0699	0.0158	0.1007	5	0.0535	0.0562	0.0212	0.0786
Nitrogen containing volatiles																	
41	Indole	120-72-9	675	1.64	1262	1273	[50, 54, 66]	5	0.0053	0.0044	0.0033	0.0080	5	0.0080	0.0088	0.0044	0.0110
42	Benzothiazole	95-16-9	618	1.58	1194	1187	[63]	5	0.0080	0.0055	0.0023	0.0154	5	0.0069	0.0054	0.0000	0.0179

a) Number of measurements taken
b) Ankle observations m=14 (not 15) due to power outages
c) First dimension retention time
d) Second dimension retention time
e) Number of days (n=5) compound was detected
f) Peak areas were normalised using the TIC of the eucalyptol IS
g) Not detected

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