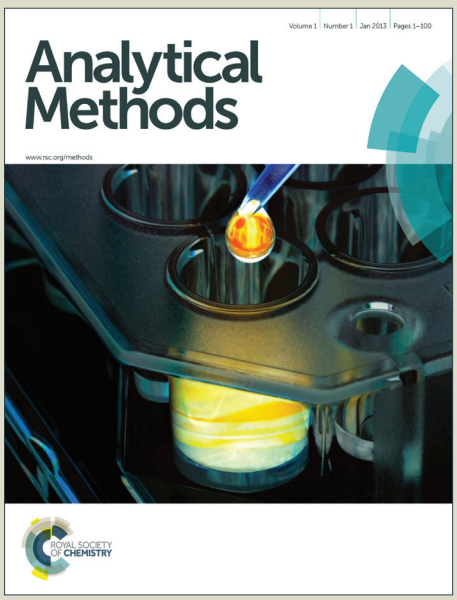
Analytical Methods

Accepted Manuscript



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Title of Manuscript: Human Body Odor Discrimination by Their GC-MS Spectra Data Mining

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Abstract

Present study explores individual identity apperception by analyzing chemical peak information in gas chromatography–mass spectrometry (GC-MS) spectra of their body odor samples with standard data mining approaches. Mainly, principal component analysis (PCA) method is opted for visual discrimination of body odor samples in feature space. PCA in combination with support vector machine (SVM) method is used for quantitative recognition. GC-MS characterization confirms composition of numerous chemical species (aldehydes, acids, ketones, esters, sulfides etc.) in body odor samples. GC-MS spectra of body odor samples from armpit and neck of three persons (with dissimilar age groups) at two different sampling times (0 h and 4 h) were recorded in experiment. Few blank (non-body odor) samples were also characterized with GC-MS and included as reference in further analysis by data mining methods. Discrimination efficiency (both qualitative and quantitative) of individual body odors were evaluated for (i) three variables of chemicals information in GC-MS spectra (peak area, peak height and ratio of peak area and height); (ii) two sampling times (0 h and 4 h); and (iii) two sampling parts of body (neck and armpit). Best visual discrimination of individual body odors has been achieved using peak height as variable for neck odor in sampling time 4 h. This result has been established with class separability measures calculated with principal component (PC) scores and SVM classification outcomes (86%).

Keywords: Body odor; GC-MS analysis; PCA, SVM; Body odor diffrentiation.

1. Introduction

Body odor is a distinguishing feature of human as well animals. It results due to secretion of water, salt, acids, oil/wax, and proteins etc. from sweat glands (*aeccrine*, *apocrine*, and *sebaceous* glands etc.) in skin and hair; in addition to exterior of epidermis layer[1-4]. Secreted compounds were metabolized by skin bacteria; in which most common types are *Brevibacterium*, *Propionibacterium acnes*, *Arcanobacterium haemolyticum*, *Micrococcus luteus*, *Staphylococcus epidermidis* etc. It results emission of characteristic odor from body; which is a complex combination of numerous species of chemicals[4,5]. Chemical species reported predominantly in literature by characterization of body odor samples are: alcohol, aldehydes, acids, amines, esters, ethers, hydrocarbon, ketones, and sulfides etc.[5-12]. Composition of chemical species in body odor alters according to parts of body such as: head, armpit, skin, breath and foot etc. Furthermore, it is affected by food and use of cosmetics, living habits and environment, diseases and emotions, genetic and age etc.[2-12]. Distinction in metabolism results a unique combination of chemical species and formation of individual odor. Distinctive attribute of individual odor has prominent impact in advanced medical, biometric, and forensic applications. Several analytical methods for characterization of body odor sample have been reported in literature. Majority of them were based on GC-MS or association of GC or MS with other instruments such as flame photometric detector, differential mobility spectrometry etc.[6-9] such as: GC-MS in characterization of feet odor samples by Kanda *et al.* identified the presence of fatty acids[6]; Headspace (HS)-GC-MS in analysis of skin odor by Haze *et al.* recognized 2-nonenal as aging biomarker[7]; Photometric detector and differential mobility spectrometry combined with GC in breath odor characterization by Muruta *et al.* and Davis *et al.* respectively[8, 9]. In addition high performance liquid chromatography (HPLC), tandem mass spectrometry (TMS), cavity ringdown

spectrometry, and atmospheric pressure ionization methods have also been used in body odor analysis[10-12] for example: cavity ringdown spectrometry which established acetone as biomarker of diabetes by Wang *et al.*[10]; atmospheric pressure ionization-MS detects acids in breath odor[11]; and HPLC-TMS in breath odor analysis by Szulejko *et al.*[12]. Research on human body odor investigation is available in many other published literatures[13-19] as well as reviewed in some reports[20, 21]. Lenochova *et al.* have described sampling methods of human body odor[22].

Characterization of body odor samples using analytical instrument like gas chromatographic mass spectrometry (GC-MS) generates enormous information (such as peak, area, peak height, ratio of area and height etc.) about the chemical species; though straight discrimination of individual on basis of their body odor spectra is not feasible. Consequently in present study, we have suggested a procedure for chemical information mining in GC-MS spectra of body odor samples for individual recognition. Statistical analysis methods have been employed in extraction of discriminating information from the massive data sets generated in characterization of body odor samples using analytical instruments. Such as principal component analysis (PCA) is used for identification of biomarker chemicals by data mining of GC-MS spectra of skin odor by Zhang *et al.*[23]; in another study by Penn *et al.*, PCA is employed in gender specific biomarker chemicals identification[24]; Chi-square test is implemented for analysis of SPME-GC-MS spectra of body odor by Spinhirne *et al.* for identification of chemicals in bovine breath[25]; Spearman correlation analysis is performed for detection of chemical compounds in analysis of SPME-GC spectra of body odor by Curran *et al.*[26]. In this context our earlier study[27] reports development of data fusion approaches for identification of discriminating body odor biomarker chemicals using kernel principal component analysis (KPCA), PCA, and majority voting methods. Except the few studies; we hardly noticed any comprehensive research based on combination of statistical

analysis methods for qualitative and quantitative discrimination of body odor samples; by mining chemical peak information in their GC-MS spectra. Moreover the performance assessment of experimental conditions such as sampling time, sampling part of body and chemical variables in GC-MS spectra on discrimination proficiency of body odor samples is also substantial.

In present study, we have used PCA for visual discrimination of body odor samples and class separability measures for their quantitative discrimination. Afterward selected features of PCA were used as input of support vector machine (SVM) classifier for quantitative (class recognition rate in percentage) recognition of individual body odor. In addition, we have assessed the performance of different chemical variables such as: peak area, peak height and ratio of peak area and height in GC-MS spectra, sampling time, and sampling part on body odor discrimination efficiency by PCA and SVM methods, independently and in combination. Detail description of experimental procedures, data analysis methods and analysis outcomes is available in subsequent sections.

2. Experimental Methods

2.1 GC-MS characterization of body odor

Present study is based on two experiments for GC-MS characterization of body odor samples in different sampling conditions. In first experiment, body odor samples were collected from three persons (say, A, B and C) instantly (sampling time 0 h). Individuals were permitted to play a baseball game for fixed time; odor samples were collected from their armpit and neck using cotton pads after finishing the game. In addition, one blank pad (without body odor) was also included for reference. Second experiment has similar conditions except the sampling time; in which body odor samples were collected from same persons and same parts of body in sampling

time 4 h (each person is asked to put cotton pads for 4 h after the baseball game). Also one blank sample was included along with the collected body odor samples similar to first experiment. By cutting each of the collected cotton pads into four parts total 24 body odor samples (3 person × 2 body parts × 4 parts of cotton pads) and 4 blank samples (1 sample × 4 parts of cotton pads) were prepared in each of the experiments. After sample collection; solid phase microextraction (SPME) technique is used for headspace generation. Samples were kept inside the SPME cells at $70^{0}C$ for 30 min to vaporize the odor molecules from body odor and blank samples. Subsequently, GC–MS with SPME auto sampler (Shimadzu QP2010) was used in characterization of odor samples (measurement time 53 min).[27, 28] Characterization of body odor extracts results record of peak area and height vs. retention time of identified chemical compounds in GC-MS spectra. Fig. 1 shows representative GC-MS spectra for armpit odor of three persons respectively (sampling time 4 h). Tables 1-4 summarize the list of chemical compounds identified in body odor samples of three persons. Three chemical variables: peak area, peak height and ratio of area and height from GC-MS spectra were selected in further data analysis.

2.2 Data matrix preparation and qualitative analysis by PCA

Composition of chemical species in body odor samples were explored by selecting fifty peaks from the GC-MS spectra of each of samples (Tables1-4). In data matrix preparation and analysis, only first 28 peaks were selected as there are only 28 body odor samples (24 body odor samples and 4 blank samples). Data matrices were prepared independently for three variables: peak area, peak height and ratio of area and height in two different sampling times (each of the data matrices of dimension 28 × 28). Detail analysis procedures are shown in Fig. 2. The first step of data analysis is logarithmic scaling; which preprocess the data matrix to reduce the weight of high valued chemical peak information. Thereafter data matrix is analyzed with PCA.

PCA is a widely used multivariate method for visualization of multidimensional data into two or three dimensional space by generating novel uncorrelated variables in feature space. In present study, PCA remodels 28-dimesional body odor samples from measurement space into principal component (PC) space. New data matrix has minimum correlation and maximum variance amongst the chemical variables (formed by the linear combination of original experimental variables i.e. chemical peak information).

After generation of novel features (PCs); selection of discriminating features is the next step of analysis. This is done by selecting first three PCs having maximum variance and discarding remaining 25 PCs. Selection of three PCs of maximum variance is convenient in reducing the noise content (contribution from additional interfering chemical compounds in peak characteristics of body odor spectra) as well visualization of body odor samples in 2-dimensional space (Figs. 3-5). Detail description of PCA method is available in refs.[29, 30]. PCA is implemented using the *'stats'* package in R (statistical computing language).[31] In addition to visual representation of body odor in PC space; a class separability measures is also introduced for quantitative differentiation of body odor samples in PC space. It assists in evaluation of minor improvement in discrimination of odor samples in PC space. Class separability index is computed in following steps (according to the ref.[30, 32]): Primarily within and between classes scatter matrices ($\mathbf{S}_w$ and $\mathbf{S}_b$) were defined as

$$\mathbf{S}_w = \sum_{i=1}^{c}\sum_{j=1}^{n}\left(p_{ij}-m_i\right)^T\left(p_{ij}-m_i\right) \quad (1)\text{, and } \mathbf{S}_b = \sum_{i=1}^{c}\left(m_i-m\right)^T\left(m_i-m\right) \quad (2)\text{, c denotes the number}$$

of classes (in present study, it is four including three persons and one blank sample), n represents total number of samples, p_{ij} is PC score of j^{th} sample belonging to i^{th} odor class, and m_i, m are the average of PC scores of i^{th} odor class and all PC scores respectively. Trace of two matrices

$\mathbf{S}_w$ and $\mathbf{S}_b$ (say $W = \text{trace}(\mathbf{S}_w)$ and $B = \text{trace}(\mathbf{S}_b)$) signify intra-classes and inter-class separability measures respectively; i.e. distribution of odor samples along the class and global mean. The class separability index (J) is defined as the ratio of inter-class and intra-classes separation as $J = B/W$. Higher value of J (i.e. higher value of B and lower value of W) indicates improved discrimination of odor samples in PC space.

2.3 Quantitative class recognition by SVM classifier

SVM method proposed by Vapnik[33] is used in machine learning for clustering, classification, regression, and anomaly detection etc. applications. In present study, SVM is used for classification of odor samples. It is a supervised classification method (includes training and validation). During the training a class separating hyperplane is formed by mapping training data set into high dimensional space through corresponding target values. Hyperplane maximizes the inter-class separation using quadratic programming and adjoining data points (support vectors). Kernel functions were proposed to reduce the computational complexity of method by computing inner product of data points in high dimensional space. Linear, Gaussian, Polynomial, Radial basis, and Sigmoid etc. are the most commonly types of used kernel functions in SVM. Decision function is formulated using the hyperplane equation and same is employed in prediction of class of an unknown odor sample in validation stage. Further mathematical details of SVM methods can be seen in refs.[29, 30, 33, 34]. We have used '*e1071*' package in R for implementation of SVM method[35].

3. Analysis Results

GC-MS characterization results of three body odor samples are presented in Figs.1 (i)-(iii). It is obvious that some chemical compounds are common and having maximum peak height and peak area; though there values are different in GC-MS spectra of individual body odor. Like in body odor spectra of person 'A' (Fig. 1 (i)); 6-methyl-5-hepten-2-one has maximum peak area 5140704 arbitrary unit (au), with peak height 1696878 au and their ratio 3.03. While for person 'B' (Fig. 1 (ii)) acetone has maximum peak area 2745397 au with peak height 203966 au and their ratio 13.46. In this case 6-methyl-5-hepten-2-one is also detected with peak area 1815175 au, peak height 589128 au and their ratio 3.08. In case of person 'C' (Fig. 1 (iii)) again acetone has maximum peak area 2263823 au with peak height 191655 au and their ratio 11.81; while 6-methyl-5-hepten-2-one has peak area 1798943 au, peak height 590797 au and their ratio 3.04. Another difference in GC-MS spectra of individual odor is due to the difference in values of peak characteristics of chemicals. Chemical compound having highest peak area may have lower peak height than the other chemicals in spectra of same person. For instance in Fig. 1(ii) acetone has maximum peak area 2745397 au but the maximum peak height is observed for the 6-methyl-5-hepten-2-one (589128 au). Accordingly GC-MS characterization of body odor samples determines only the composition of chemical compounds absolutely. Due to complex composition of chemical compounds and their correlation; discrimination of individual directly on basis of peak characteristics of GC-MS spectra of their body odor is not feasible. Statistical analysis is essential to find the discriminating characteristics of chemical compounds for individual differentiation. PCA and SVM methods were selected for visual and quantitative discrimination of individual using peak characteristics of chemical in GC-MS spectra of their body odor. Analysis procedures are given in Fig. 2. In first step, six different data matrices were

prepared using peak area, peak height and ratio of peak area and height as variables for 28 samples (24 body odor and 4 blank samples) in two different sampling times (0 h and 4 h). After that each of the data matrices were preprocessed using the logarithmic scaling; which reduces the effect of very high or very low value of any of three variables on further analysis outcomes. PCA is used in transformation of body odor data from experimental space to feature space. 28-dimesional feature vectors were generated by PCA. Out of which only first three dimensions having maximum values of variance were selected in visual representation of body odor samples in 2-dimensional feature space (Figs. 3-5). Particularly, Figs. 3 (a)-(c) represent body odor and blank samples in PC 1-2 dimensional space using peak area, peak height and ratio of peak area and height as variables for sampling time 0 h (instant sample collection) respectively. Similar, representation of body odor and blank samples for data matrices of sampling time 4 h is given in Figs. 3 (d)-(f) using three variables peak area, peak height and ratio of peak area and height respectively. To check the impact of sampling parts of body on individual discrimination; PCA outcome is shown in Figs. 4 (a), and 4 (b) which represents discrimination of body odors and blank samples using peak area as variable in sampling time 4 h from armpit and neck respectively. Individual discrimination results using peak height as variable and sampling time 4 h with armpit and neck odor respectively is given in Figs. 4 (c), and 4 (d); while Figs. 4 (e), and 4 (f) represent individual discrimination using the ratio of peak area and height in similar conditions. Discrimination of blank sample, armpit odor and neck odor of all subjects in sampling time 4 h and using peak area as variable is shown in Fig. 5. PCA results (Figs. 3-5) evaluate the effect of sampling time, sampling parts and chemical peak information on individual odor discrimination. Next, PC scores were used as input of SVM classifier for quantitative recognition of individual body odor summarized in Tables 5, and 6. Particularly, left part of

Table 5 presents class confusion matrix of SVM classification for PC scores (Fig. 3 (a)-(c)) of GC-MS spectra data in sampling time 0 h using peak area, peak height and ratio of peak area and height as variables respectively. Out of total 28 samples (24 body odor samples and 4 blank samples); 21 samples (18 body odor samples (6 from each person) and 3 blanks samples) were used in training of SVM model. Rest 7 samples (6 body odor samples (2 from each person) and 1 blank sample) were used in validation. Using the PC scores of GC-MS spectra data in sampling time 4 h and peak area, peak height and ratio of peak area and height as variables respectively (Figs. 3 (d)-(f)); SVM classification performance for individual body odor discrimination is given in right part of Table 5. To check the effect of odor sampling parts (armpit and neck) on individual odor discrimination efficiency by SVM classifier; PC scores of GC-MS spectra data matrix in sampling time 4 h using peak area as variable (Figs. 4 (a), and 4 (b)) is used in input of SVM classifier. In this case 12 samples (9 body odor samples (3 from each person) and 3 blanks samples) were used in training of SVM model. Rest 4 samples (3 body odor samples (1 from each person) and 1 blank sample) were used in validation. Classification performance in individual body odor discrimination with validation data set is shown in Table 6. SVM classification results in similar sampling condition but using the PC scores of peak height and ratio of peak area and height as variables (Figs. 4 (c), 4 (d), and 4 (e), 4 (f)) with validation data sets are also presented in Table 6. In case of SVM classification results using the PC scores corresponding to Fig. 5 for discrimination of blank samples and parts of body odor on the basis of their GC-MS spectra with validation samples is as follows: total 21 samples (18 body odor samples (9 from each body part including the armpit and neck, and 3 blanks samples) were used in training of SVM model, rest 7 samples (6 body odor samples (3 from each body part, and 1 blank sample) are used in validation. It results correct identification of 6 out of 7 odor samples.

4. Discussion

GC-MS characterization results of body odor samples are detailed in Figs. 1(i)-(iii), and in Tables1-4. It is obvious that body odor samples have complex composition of several chemical species in GC-MS spectra. There are some common, besides characteristics chemical compounds in individual odor samples. For instance comparing the armpit odor composition of three persons; there are 18 common chemical compounds such as: Acetone, Octamethyl-Cyclotetrasiloxane, Trimethyl-Silanol, 2-Ethoxyethyl acetate, Decanal, 2-Methyl-2-propenoic acid etc. besides; other characteristics chemical compounds are Dodecane, Hexadecane, 2-Decenol, Isomenthol, Octadecamethyl-Cyclononasiloxane etc. in person 'A'; 3-Butynol, Topotecan, Dodecanal, 5-Propyl-decane etc. in person 'B'; and 1, 2-Propadiene-1, 3-dione, Toluene, Hexanal, Heptanal, Nonanal etc. in person 'C' respectively (Tables 1-3). There are some common chemical compounds in armpit odor of two persons such as: 2-Formylhistamine, Acetic acid, Methoxy-phenyl-oxime etc. in persons 'A' and 'C'. In addition there is also difference in chemical composition of odor samples from different parts of body as well in different sampling time of same person. Like in case of person 'A' some common chemical compounds detected in armpit and neck odor are: Acetone, Octamethyl-Cyclotetrasiloxane, Trimethyl-Silanol, 2-Formylhistamine, 2-Methyl-2propenoic acid, Methoxy-phenyl-oxime, etc. besides characteristics chemicals such as: Dodecane, Hexadecane, Tetradecane, Decanal, Lilial etc. and Heptanal, Nonanal, Dodecanal, 2, 2-oxybis-Ethanol, etc. were detected in armpit and neck odor respectively (Table-1). Effects of chemical composition of body odor samples from armpit of person 'A' due to difference in sampling time is obvious from the Table-4. There are few common chemicals in sampling time 0 h and 4 h such as 6-Methyl-5-hepten-2-one, 1, 3-dihydroxy-2-propanone, Dimethyl-Silanediol, N, N-dibutyl-Formamide, etc. Dissimilar chemical

compounds in sampling time 4 h compare to instant sampling 0 h is due to chemical and biological decomposition activities of skin bacterial. Merely, observation of common and characteristics chemical compounds in body odor composition is not enough to find out the discriminating information of individual. For that reason, statistical data mining protocol is adopted in analysis of body odor composition for extracting discriminating information of individual body odor (Fig. 2). Figs. 3 and 4 present qualitative representation of individual body odor discrimination in feature space. Besides the qualitative discrimination of body odor samples by visual assessment; class separability index J (ratio of between class B and within class separation W) [20, 24] is computed in each case for quantitative assessment. Comparing the performance of chemical peak information such as area, height and ratio of area and height on odor discrimination in sampling time 0 h is demonstrated in Figs. 3 (a)-(c) respectively. Visual inspection reveals the formation of 4, 3 and 2 hypothetical odor clusters in PC space using peak area, peak height and their ratio as variables respectively. With decrease in number of clusters; misclassifications amongst the body odor as well blank samples also increases. This fact is further verified with the maximum value of class separability index $J = 0.019$ for peak area variable. Performance comparison of chemical peak information on odor discrimination in sampling time 4 h is demonstrated in Figs. 3 (d)-(f) respectively. In this case 4, 3, 3 hypothetical odor clusters were identified in PC space for peak area, height and their ratio as variables respectively. Similar to sampling time 0 h the maximum discrimination $(J = 0.033)$ amongst the body odor and blank samples has been achieved using chemical peak area information; while the ratio of peak area and height results maximum overlapping $(J = 0.011)$. Visual inspections of PC score plots in Figs. 3 (a-c), and (d)-(f) and class separability measures in each case affirm the high impact of sampling time 4 h than 0 h on body odor discrimination. Furthermore better

performance of chemical peak area information compare to peak height and ratio of peak area and height is obvious in both 0 h and 4 h sampling time experiments. Chemical peak information of sampling time 4 h is utilized further in analysis to check the impact of sampling part of body (neck and armpit) on individual odor discrimination in PC space (Figs. 4 (a)-(f)). Assumed odor clusters, using chemical peak area for body odor samples collected from armpit and neck are shown in Figs. 4 (a), and 4 (b) respectively. Both the visual inspection and quantitative class separability measures confirm better performance of neck odor than armpit odor in individual odor discrimination. Similar results were obtained using chemical peak height and ratio of area and height information analysis (shown in Figs. 4 (c), 4 (d), and 4 (c), 4 (d) respectively). Best visual discrimination amongst the individual and blank samples and maximum class separability index $(J = 0.90)$ is achieved for neck odor using the chemical peak height information (Fig. 4 (d)). Differentiation results of neck and armpit odor with blank samples for all the subjects are demonstrated in Fig. 5. Blank samples were completely separated with body odors while few neck odors overlap with armpit odors samples, which results low value of class separability index $(J = 0.065)$ for three odor clusters. Individual odor recognition results of SVM, using PC scores in Figs. 3 (a)-(c) for validation data set are summarized in left part of Table 5. Maximum recognition rate (57%) is achieved using chemical peak area information; while ratio of peak area and height results minimum recognition rate (14%). SVM classification results are in agreement with the visual and class separability measure results in PCA analysis (Figs. 3 (a)-(c)) as peak area results maximum while ratio of peak area and height results minimum class discrimination in PC space. PC scores of body odor data in sampling time 4 h (Fig. 3 (d)-(f)) results better class recognition by SVM for validation data set as shown in right part of Table 5 compare to 0 h sampling experiment in left part of Table 5. Again, chemical peak area

information results maximum class recognition rate (86%); while the ratio of area and height results minimum class recognition rate (43%). SVM class recognition results support PCA results in Fig. 3 (d)-(f). Consequently, SVM classification results in Table 5 validate the better performance of sampling time 4 h compare to 0 h and chemical peak area information compare to peak height and ratio of area and height on body odor discrimination similar to PCA results in Figs. 3 (a)-(f). SVM classification results for performance assessment of sampling parts of body on individual odor discrimination using the PC scores (Figs. 4 (a)-(f)) are shown in Table 6. SVM classification results reveal better performance of neck odor compare to armpit odor in body odor discrimination for each of the three chemical peak variables, similar to PCA results shown in Figs. 4 (a)-(f). In this case, maximum class recognition rate (75%) is achieved for the neck odor using the peak height information of chemicals. For identification of odor from neck and armpit of all the subjects, PC scores in Fig. 5 were used in input of SVM model. SVM results 86% correct class recognition rate.

5. Conclusion

We studied recognition of individual body odors and discrimination with non-body odor samples by their GC-MS characterization and further data mining approaches (PCA and SVM). Effect of sampling time, chemical information in GC-MS spectra, and sampling parts on identification of individual body odors and their differentiation with non-body odor samples are demonstrated in detail. Performance of analysis outcome is estimated by visual inspection of odor and non-odor samples in PC space, their class separability measures, and SVM classification results. Better recognition and discrimination results are accomplished with sampling time 4 h compare to 0 h, neck odor compare to armpit odor, and peak area compare to

peak height, and ratio of area and height. Though the chemical peak height of neck odor in sampling time 4 h results best clustering of body odors of three persons and blank samples as well their maximum class recognition (86%) by SVM classifier. Present study includes limited subjects in body odor experiments, though number of samples is increased by collecting samples at different times, and parts of body. In future, we target to collect body odor samples in advance controlled environment from more subjects as well develop efficient data mining approaches for their odor identification using chemical peak information from GC-MS spectra.

Acknowledgements

The author S.K.J. gratefully acknowledges all the lab colleagues and Mrs. Anju Sunil Jha and Dr. S.S. Murthy (Assistant Director, CFSL, Hyderabad, India) for their cooperation and support during the study.

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Table Captions

Table 1 Chemical compounds detected in body odor of person 'A' by selecting 50 peaks in GC-MS spectra.

Table 2 Chemical compounds detected in body odor of person 'B' by selecting 50 peaks in GC-MS spectra.

Table 3 Chemical compounds detected in body odor of person 'C' by selecting 50 peaks in GC-MS spectra.

Table 4 Comparative list of chemical compounds found in armpit odor of person 'A' at two different sampling times by selecting 50 peaks in GC-MS spectra.

Table 5 SVM classification results for body odor experiments with sampling time 0 h and 4h.

Table 6 SVM classification results for body odor samples using PC scores of peak area, peak height and ratio of peak area and height in their GC-MS spectra (sampling time 4 h).

Figure Captions

Fig. 1 GC-MS spectra of armpit odor in sampling time 0 h from person (i) A, (ii) B, and (iii) C.

Fig. 2 Schematic steps in analysis of body odor data from their GC-MS spectra.

Fig. 3 PCA score plots using (a) peak area, (b) peak height, and (c) ratio of peak area and height as variable (sampling time 0 h); and (d) peak area, (e) peak height, and (f) ratio of peak area and height as variable (sampling time 4 h) in body odor data analysis.

Fig. 4 Person differentiation using PC scores of (a) armpit odor, (b) neck odor (peak area as variable); (c) armpit odor, (d) neck odor (peak height as variable); (e) armpit odor (f) neck odor (ratio of peak area and height as variable) sampling time 4 h in all cases.

Fig. 5 Differentiation of body odor samples from armpit and neck on the basis of PC scores by analysis of body odor experiment data with sampling time 4 h and using peak area as variable.

Table 1

Armpit Odor	Neck Odor
Argon	3-Butyn-1-ol
Acetone	1,2-Propadiene-1,3-dione
Cyclotetrasiloxane, octamethyl-	Acetone
Silanol, trimethyl-	Cyclotetrasiloxane, octamethyl-
2-Formylhistamine	Silanol, trimethyl-
Cyclopentasiloxane, decamethyl-	2-Formylhistamine
Dodecane	Cyclopentasiloxane, decamethyl-
1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane	2-Propanol, 1-methoxy-
Cyclohexasiloxane, dodecamethyl-	Heptanal
Nonane, 2,2,4,4,6,8,8-heptamethyl-	1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane
Hexadecane	D-Limonene
2-Ethoxyethyl acetate	Cyclohexasiloxane, dodecamethyl-
5-Hepten-2-one, 6-methyl-	Methoxyacetic acid, 3-tridecyl ester
Tetradecane	2-Ethoxyethyl acetate
2,2-Dimethyl-1-pentamethyldisilanyloxypropane	5-Hepten-2-one, 6-methyl-
2-Decen-1-ol, (E)-	Tetradecane
Acetic acid	Nonanal
1-Hexanol, 2-ethyl-	Formamide, N,N-diethyl-
Decanal	Dodecanal
Cyclooctasiloxane, hexadecamethyl-	Acetic acid
Cyclohexanol, 2-(1,1-dimethylethyl)-	1-Hexanol, 2-ethyl-
2-Propanone, 1,3-dihydroxy-	Decanal
Silanediol, dimethyl-	Cyclooctasiloxane, hexadecamethyl-
(+)-Isomenthol	Pyrimidine-2,4(1H,3H)-dione, 5-amino-6-nitroso-
Cyclononasiloxane, octadecamethyl-	Silanediol, dimethyl-
2-Propenoic acid, 2-methyl-	Menthol
Oxime-, methoxy-phenyl-_	2-Propenoic acid, 2-methyl-
Formamide, N,N-dibutyl-	Oxime-, methoxy-phenyl-_
Heptasiloxane, hexadecamethyl-	Formamide, N,N-dibutyl-
2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester	2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
Butylated Hydroxytoluene	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester
Cyclooctasiloxane, hexadecamethyl-	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
Hexanoic acid, 2-ethyl-	Hexanoic acid, 2-ethyl-
1-Dodecanol	1-Dodecanol
Indan-1,3-diol monopropionate	Ethanol, 2,2'-oxybis-
Lilial	1,4-Benzenediol, 2-[(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)methyl]-, [1R-(1.alpha.,4a.beta.,8a.alpha.
1,4-Benzenediol, 2-[(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)methyl]-, [1R-(1.alpha.,4a.beta.,8a.alpha.	Hexane, 1,2,3-trimethoxy-
2-[2-[2-[2-[2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	Phenol, 2,6-bis(1,1-dimethylethyl)-
1,3-Pentanediamine	Heptanal dipropyl acetal
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, [S-(Z)]-	1,4,7,10,13,16-Hexaoxanonadecane, 18-(2-propenyl)-
Phenol, 2,4-bis(1,1-dimethylethyl)-	9,12-Octadecadienoic acid, methyl ester, (E,E)-
3-Hexene, 1-[1-ethoxyethoxy]-, (E)-	9-Decen-1-yl acetate
2-(p-Tolylmethyl)-p-xylene	cisZ-11,12-Epoxytetradecan-1-ol
9-Decen-1-ol, methyl ether	Octanal, 2-(phenylmethylene)-
1-Methoxy-3-(2-hydroxyethyl)nonane	4-Methylmannitol
Octanal, 2-(phenylmethylene)-	Glycylglycine ethyl ester
12-Crown-4	15-Crown-5
N-t-Butyl-N'-[1,1-dimethyl-2-thiosulfatoethyl]-1,3-	1-Propanol, 2-(2-methoxy-1-methylethoxy)-

propanediamine

Table 2

Armpit Odor	Neck Odor
l-Alanine ethylamide, (S)-	dl-Alanyl-l-alanine
3-Butyn-1-ol	3-Butyn-1-ol
3-Butyn-1-ol	Cyclopentasiloxane, decamethyl-
Acetone	Dodecane
Cyclotrisiloxane, hexamethyl-	1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane
Isopropyl Alcohol	Cyclohexasiloxane, dodecamethyl-
Ethanol	Tetradecane
Cyclotetrasiloxane, octamethyl-	2-Ethoxyethyl acetate
Silanol, trimethyl-	Cyclotrisiloxane, hexamethyl-
Topotecan	5-Hepten-2-one, 6-methyl-
Cyclopentasiloxane, decamethyl-	Piperidine, 3,3-dimethyl-
2-Propanol, 1-methoxy-	Tetradecane
1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane	Nonanal
Cyclohexasiloxane, dodecamethyl-	Formamide, N,N-diethyl-
Decane, 5-propyl-	Hexadecanal
2-Ethoxyethyl acetate	1-Hexanol, 2-ethyl-
5-Hepten-2-one, 6-methyl-	Decanal
Tetradecane	Cyclooctasiloxane, hexadecamethyl-
Cycloheptasiloxane, tetradecamethyl-	2-Propanone, 1,3-dihydroxy-
Dodecanal	Silanediol, dimethyl-
1-Hexanol, 2-ethyl-	Cyclononasiloxane, octadecamethyl-
Decanal	2-Propenoic acid, 2-methyl-
Cyclooctasiloxane, hexadecamethyl-	Formamide, N,N-dibutyl-
2-Propanone, 1,3-dihydroxy-	2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester
Silanediol, dimethyl-	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
2-Propenoic acid, 2-methyl-	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
Formamide, N,N-dibutyl-	1-Dodecanol
2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester	3-Methyloxirane-2-carboxylic acid
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	Butane, 2-ethoxy-
N,N-Dimethylbutyramide	1,4,7,10,13,16-Hexaoxacyclooctadecane
(4-Acetylphenyl)phenylmethane	Phenol, 2,6-bis(1,1-dimethylethyl)-
1-Nitro-2-acetamido-1,2-dideoxy-d-glucitol	Tetraethylene glycol diethyl ether
1,6-Dideoxy-l-mannitol	Propane, 2,2'-[ethylidenebis(oxy)]bis-
1-Butene, 3,3-bis[[(tert-butyldimethylsilyl)oxy]methyl]-4-[(2-methoxyethoxy)methoxy]-	Propane, 2-ethoxy-
2-[2-(2-Ethoxyethoxy)ethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate	N-Ethyl-N-nitroso-N'-nitroguanidine
2-[2-[2-[2-[2-[2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	2-Aminooxy-4-methylvaleric acid, methyl ester
1,1'-Biphenyl, 2,2',5,5'-tetramethyl-	1,4,7,10,13,16-Hexaoxacyclooctadecane
Ethane, 1,1'-oxybis[2-ethoxy-]	2,3-Butanediol, 1,4-dimethoxy-
2-[2-[2-[2-[2-[2-[2-[2-[2-(Trimethylsilyloxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	Ethanol, 2-(2-methoxyethoxy)-
1-Methoxy-3-trimethylsilyloxymethyloctane	1,3-Dioxolane, 2,4,5-trimethyl-
N-Acetyl-.alpha.-aminooxybutyric acid, methyl ester	1,4-Dioxan-2-ol
Methyl 3-O-acetyl-2,4,6-tri-O-methyl-.alpha.-D-glucopyranoside	Heptanoic acid, 2-methyl-6-oxo-, methyl ester
2,5,8,11,14-Pentaoxahexadecan-16-ol	1,6-Dideoxy-2,4-monoethylene-d-altritol
15-Crown-5	1,4,7,10,13,16-Hexaoxacyclooctadecane
1,4,7,10,13,16-Hexaoxacyclooctadecane	Heptane, 4-methoxy-3-(methoxymethyl)-
R-(+)-Methyl-3-isopropyl-6-oxoheptanoate	Acetoacetic acid, 1,3-dithio-, S-propyl ester
tert-Butyl-[2-[2-[2-(2-butoxyethoxy)ethoxy]ethoxy]ethoxy]dimethylsilane	Ethane, 1,1'-oxybis[2-ethoxy-]
Pentaethylene glycol	1,4,7,10-Tetraoxa-13-azacyclopentadecane
1,2-Propanediol, 3-methoxy-	3-Hexanol, 3-ethyl-

N,N-Dimethylsuccinamic acid	3,6,9,12-Tetraoxatetradecan-1-ol

Table 3

Armpit Odor	Neck Odor
1,2-Propadiene-1,3-dione	Argon
Acetone	Azetidin-2-one 3,3-dimethyl-4-(1-aminoethyl)-
Cyclotrisiloxane, hexamethyl-	m-Dioxan-4-ol, 2,6-dimethyl-
Isopropyl Alcohol	Allene
Ethanol	Propanal, 2,2-dimethyl-, oxime
Cyclotetrasiloxane, octamethyl-	Propanamide, 2-methyl-
1R-.alpha.-Pinene	Dimethylamine
Silanol, trimethyl-	cis-Aconitic anhydride
Toluene	1,4,7,10,13,16-Hexaoxacyclooctadecane
2-Formylhistamine	Argon
Hexanal	Acetone
Cyclopentasiloxane, decamethyl-	Cyclotrisiloxane, hexamethyl-
Heptanal	Isopropyl Alcohol
1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane	Ethanol
3-Cyclohexyl-1-propyne	Cyclotetrasiloxane, octamethyl-
Cyclohexasiloxane, dodecamethyl-	Silanol, trimethyl-
2-Ethoxyethyl acetate	Toluene
5-Hepten-2-one, 6-methyl-	2-Formylhistamine
Tetradecane	Cyclopentasiloxane, decamethyl-
Nonanal	1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane
Formamide, N,N-diethyl-	Cyclohexasiloxane, dodecamethyl-
.alpha.-Methyl-.alpha.-[4-methyl-3-pentenyl]oxiranemethanol	Tridecane
Acetic acid	2-Ethoxyethyl acetate
.alpha.-Methyl-.alpha.-[4-methyl-3-pentenyl]oxiranemethanol	5-Hepten-2-one, 6-methyl-
1-Hexanol, 2-ethyl-	Tetradecane
Decanal	Nonanal
Cyclooctasiloxane, hexadecamethyl-	Formamide, N,N-diethyl-
2-Propanone, 1,3-dihydroxy-	1-Hexanol, 2-ethyl-
Silanediol, dimethyl-	Decanal
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1.alpha. 2. beta., 5.alpha.)-	Pyrimidine-2,4(1H,3H)-dione, 5-amino-6-nitroso-
1-Nonanol	Silanediol, dimethyl-
2-Propenoic acid, 2-methyl-	2-Propenoic acid, 2-methyl-
Oxime-, methoxy-phenyl-_	Tetradecanal
Formamide, N,N-dibutyl-	Formamide, N,N-dibutyl-
2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	1-Dodecanol
Hexanoic acid, 2-ethyl-	3,4,6-Tri-O-methyl-d-glucose
1-Dodecanol	Heptaethylene glycol
1,3,4-Trimethoxy-butan-2-ol	Propane, 1,3-dimethoxy-
2-[2-(2-Butoxyethoxy)ethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hydroxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol
2-(p-Tolylmethyl)-p-xylene	1,1'-Biphenyl, 2,2',5,5'-tetramethyl-
tert-Butyl-[2-(2-ethoxyethoxy)ethoxy]dimethylsilane	Oxirane, (ethoxymethyl)-
1,4-Butanediamine, N-(3-aminopropyl)-	L-Glucose
Ethanol, 2-[2-(2-ethoxyethoxy)ethoxy]-	Ethanol, 2,2'-[oxybis(2,1-ethanediyloxy)]bis-
1,4,7,10,13,16,19-Heptaoxa-2-cycloheneicosanone	L-Cysteine, N-acetyl-, methyl ester, acetate
N-Methoxy-2-carbomethoxyaziridine	S-[2-Aminoethyl]-dl-cysteine
2-[2-[2-[2-[2-[2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethanol	Butane, 1,2,4-trimethoxy-
Butanoic acid, 3-hydroxy-, ethyl ester	Carbamic acid, dimethyl-, ethyl ester
d-Gluconic acid dimethylamide	Octanal, 2-(phenylmethylene)-
2-[2-[2-[2-[2-[2-[2-[2-(2-	Methoxyacetic acid, cyclobutyl ester

Hydroxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]ethoxy]etho xy]ethanol

Table 4

Sampling time 0 h	Sampling time 4 h
Butanoic acid, 3-chloro-	Acetone
Acetic acid, oxo-	Cyclotrisiloxane, hexamethyl-
1,2-Propadiene-1,3-dione	Cyclotetrasiloxane, octamethyl-
4-(2-Hydroxyethylamino)-3-nitrocoumarin	Silanol, trimethyl-
Argon	Hexanal
3-Butyn-1-ol	Cyclopentasiloxane, decamethyl-
Argon	Heptanal
Argon	Dodecane
Argon	1,3-Diisopropoxy-1,3-dimethyl-1,3-disilacyclobutane
Argon	Cyclohexasiloxane, dodecamethyl-
4-Spirohexanone, 5,5-dichloro-	Nonane, 2,2,4,4,6,8,8-heptamethyl-
Cyclopropene	Octanal
8,9,9,10,10,11-Hexafluoro-4,4-dimethyl-3,5-dioxatetracyclo[5.4.1.0(2,6).0(8,11)]dodecane	2-Ethoxyethyl acetate
Argon	5-Hepten-2-one, 6-methyl-
2-Ethyl(dimethyl) silyloxydodecane	Tetradecane
2,4(1H,3H)-Pyrimidinedione, dihydro-5-hydroxy-	Nonanal
1H-Pyrrole, 2,5-dihydro-1-nitroso-	.alpha.-Methyl-.alpha.-[4-methyl-3-pentenyl]oxiranemethanol
1,2,3-Butanetriol	Dodecanal
dl-Threonine, methyl ester	Acetic acid
5-Hepten-2-one, 6-methyl-	.alpha.-Methyl-.alpha.-[4-methyl-3-pentenyl]oxiranemethanol
Acetic acid	1-Hexanol, 2-ethyl-
3-Bromo-2-prop-1-ynyltetrahydrofuran	Decanal
2-Butanone	Cyclooctasiloxane, hexadecamethyl-
2-Heptanol, 5-ethyl-	Cyclohexanol, 2-(1,1-dimethylethyl)-
Decanal	Octane, 2,4,6-trimethyl-
Propanoic acid	2-Propanone, 1,3-dihydroxy-
Dimethyl Sulfoxide	Silanediol, dimethyl-
2-Propanone, 1,3-dihydroxy-	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1.alpha.,2.beta.,5.alpha.)-
Silanediol, dimethyl-	4-tert-Butylcyclohexyl acetate
Hexanoic acid	Formamide, N,N-dibutyl-
Formamide, N,N-dibutyl-	cis-syn-trans-Tricyclo[7.3.0.0(2,6)]dodec-7-ene
2-Propenoic acid, 2-methyl-, 2-hydroxyethyl ester	2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester
Imidazole, 5-fluoro-1-ribofuranosyl-	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
2-Propenoic acid, 2-methyl-, 1,2-ethanediyl ester	.alpha. Isomethyl ionone
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester
2,5-Isoxazolidinedicarboxylic acid, 2-ethyl 5-methyl ester	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester
Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester	Pyrazole-3-carboxylic acid, 1-(1-adamantyl)-4-nitro-
1,6-Dideoxy-2,4-monoethylene-d-altritol	Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl ester
Ethanol, 2,2'-oxybis-	Butylated Hydroxytoluene
Phenol	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
Ethanol, 2-phenoxy-	Hexanoic acid, 2-ethyl-
4,8,12-Tetradecatrienal, 5,9,13-trimethyl-	1-Dodecanol
15-Crown-5, [2-(diethylboryl)phenyl]-	Bicyclo[3.2.0]hept-2-ene, exo-4-tert.butoxy-
Triethylene glycol	1-Heptadecanamine, N,N-dimethyl-
7-Triethylsilyloxytridecane	Lilial
dl-Homocysteine	1,4-Benzenediol, 2-[(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)methyl]-, [1R-(1.alpha.,4a.beta.,8a.alpha.
Cycloserine	(7a-Isopropenyl-4,5-dimethyloctahydroinden-4-yl)methanol
Pentane, 1-(propylthio)-	12,15-Octadecadienoic acid, methyl ester
Trans-2,3-dimethylthiane	11,14-Eicosadienoic acid, methyl ester

Ethanol, 2-(2-ethoxyethoxy)-	Octanal, 2-(phenylmethylene)-

Table 5

Data from body odor experiments with sampling time 0 h	Data from body odor experiments with sampling time 4 h
Based on PC scores of peak area Predicted class True class 0 0 1 0 0 1 0 1 0 0 1 1 0 0 0 2 4 samples identified out of 7	Based on PC scores of peak area Predicted class True class 0 0 1 0 0 2 0 0 0 0 2 0 0 0 0 2 6 samples identified out of 7
Based on PC scores of peak height Predicted class True class 0 0 0 1 0 1 0 1 0 0 0 2 0 0 1 1 2 samples identified out of 7	Based on PC scores of peak height Predicted class True class 1 0 0 0 1 1 0 0 0 0 1 1 0 0 0 2 5 samples identified out of 7
Based on PC scores of ratio of peak area and height Predicted class True class 0 1 0 0 0 1 0 1 0 1 0 1 0 2 0 0 1 samples identified out of 7	Based on PC scores of ratio of peak area and height Predicted class True class 0 1 0 0 0 2 0 0 0 1 0 1 0 1 0 1 3 samples identified out of 7

Table 6

Classification results based on PC scores of peak area (sampling time 4 h)

Person identification using armpit odor

True class \ Predicted class				
	1	0	0	0
	0	0	0	1
	0	0	1	0
	0	0	1	0

2 samples identified out of 7

Person identification using neck odor

True class \ Predicted class				
	1	0	0	0
	0	0	0	1
	0	0	1	0
	0	0	1	0

2 samples identified out of 7

Classification results based on PC scores of peak height (sampling time 4 h)

Person identification using armpit odor

True class \ Predicted class				
	1	0	0	0
	0	0	0	1
	0	0	0	1
	0	1	0	0

1 samples identified out of 7

Person identification using neck odor

True class \ Predicted class				
	1	0	0	0
	0	1	0	0
	0	0	1	0
	0	1	0	0

3 samples identified out of 7

Classification results based on PC scores of ratio of peak area and height(sampling time 4 h)

Person identification using armpit odor

True class \ Predicted class				
	0	1	0	0
	0	0	0	1
	0	0	0	1
	0	0	0	1

1 samples identified out of 7

Person identification using neck odor

True class \ Predicted class				
	1	0	0	0
	0	1	0	0
	1	0	0	0
	0	1	0	0

2 samples identified out of 7

Fig. 1

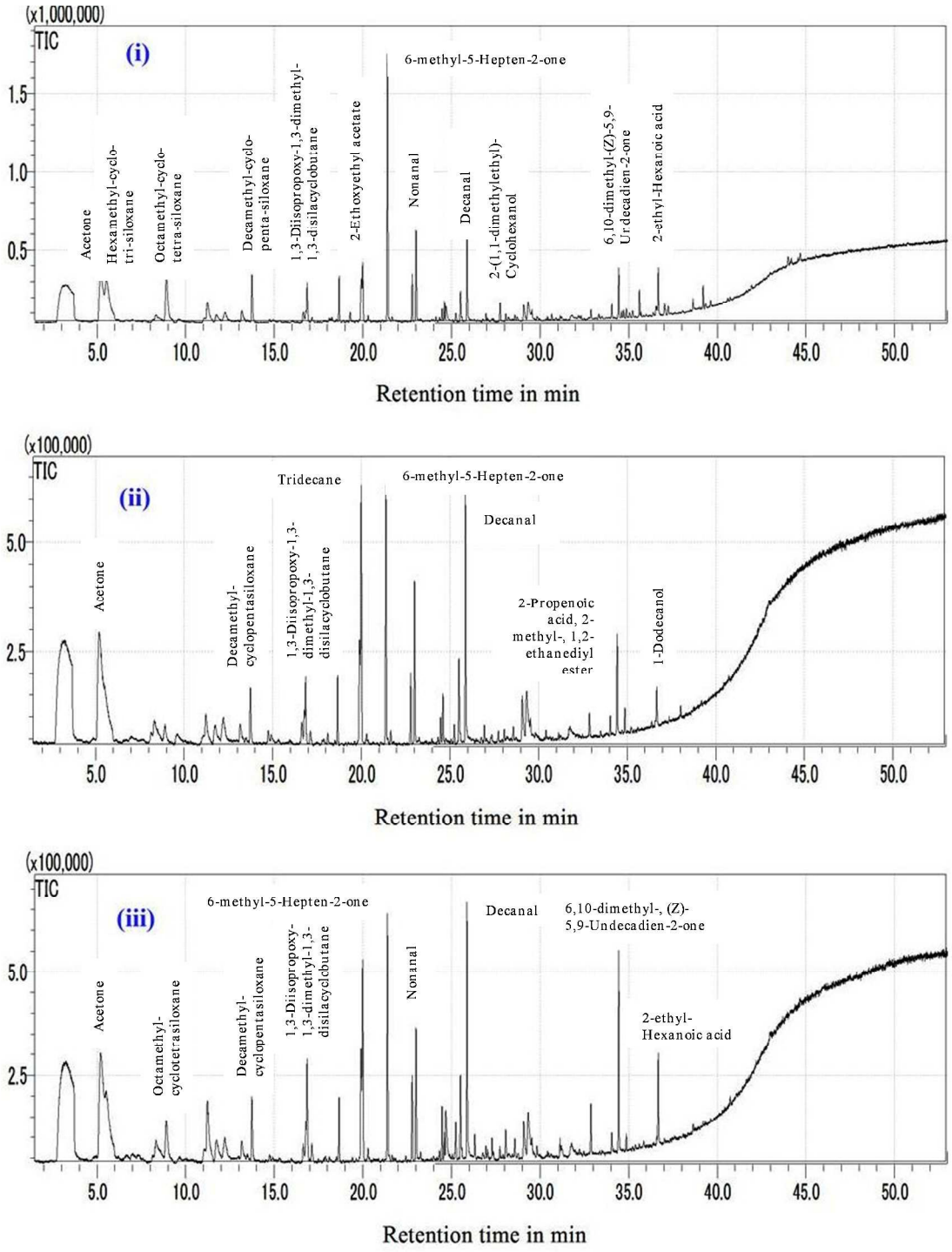

Fig. 2

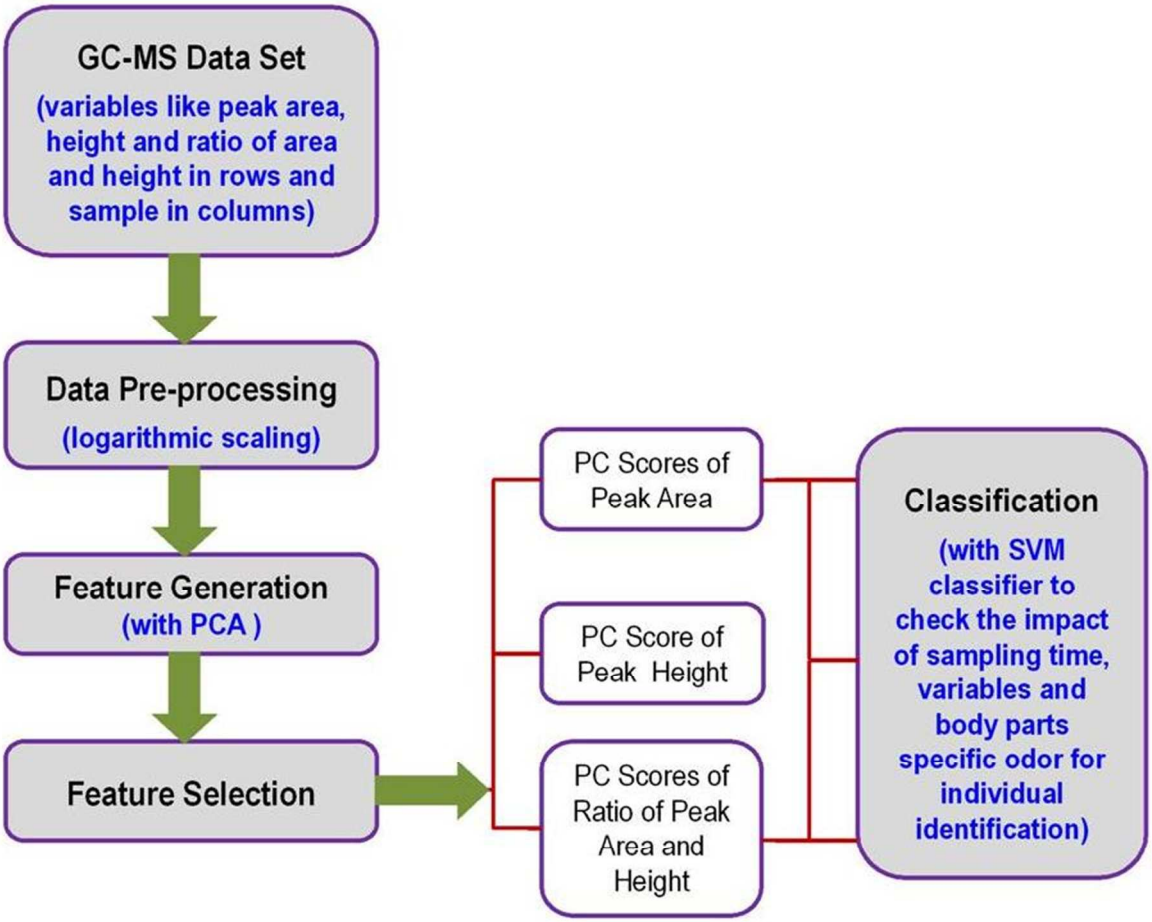

Fig. 3

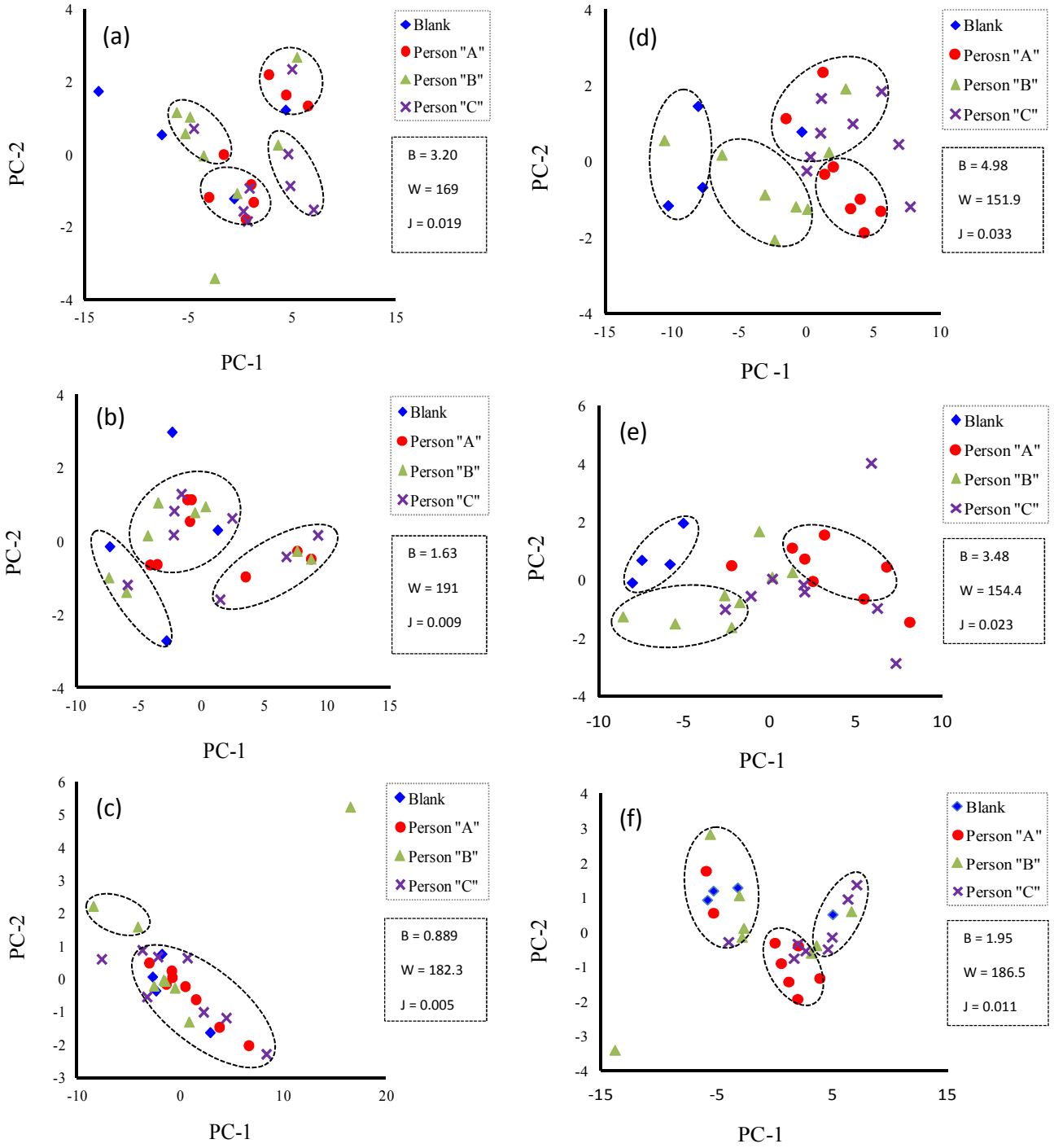

Fig. 4

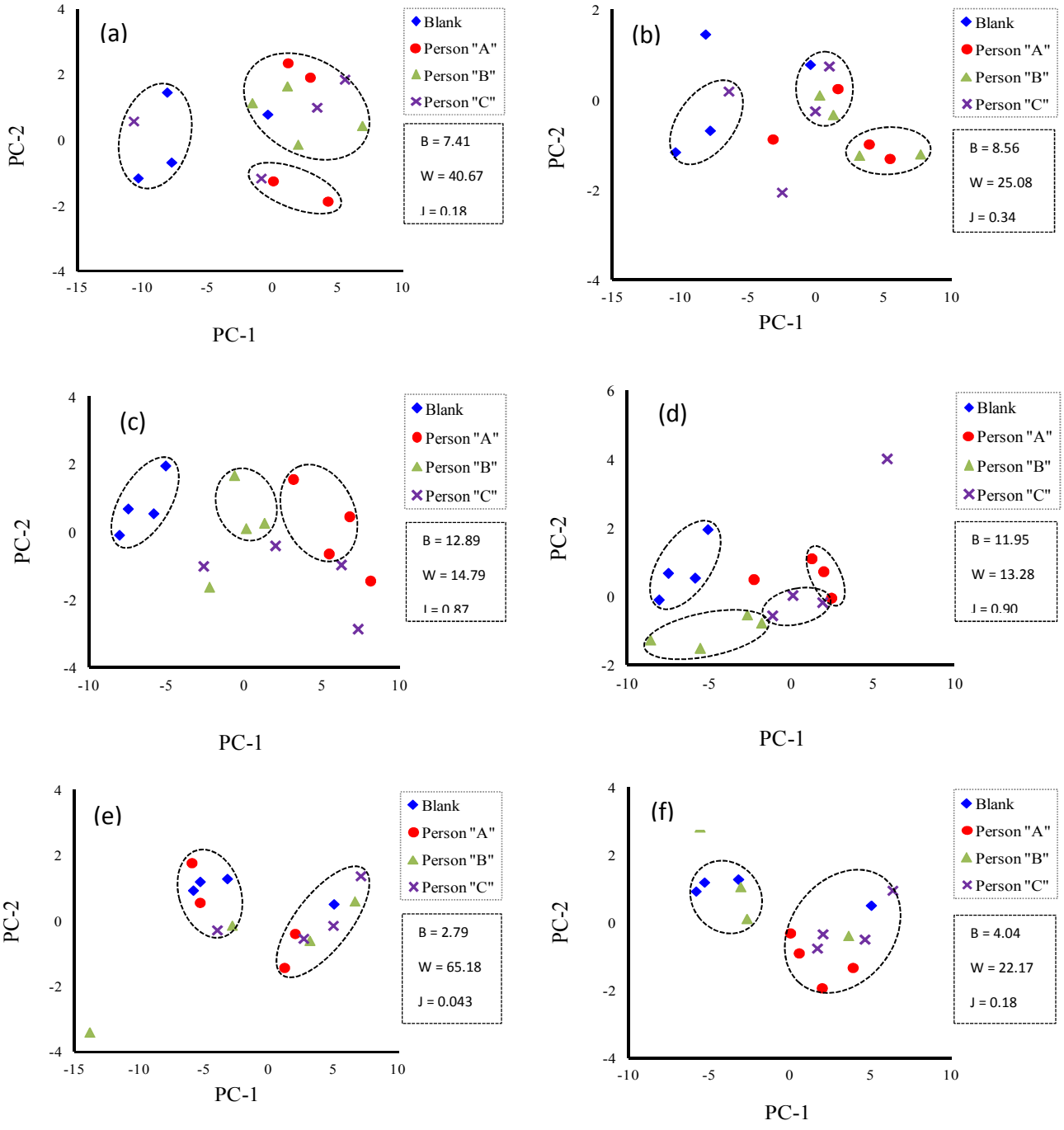

Fig. 5