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Characterization of human body odor and identification of aldehydes using chemical sensor

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Abstract: Human body odor is a unique identity feature of individual as well as an established composite of numerous volatile organic compounds (VOCs) belonging to significant chemical classes. Several analytical methods have been used in the characterization of human body odor in order to recognize the chemical composition of VOCs in medical, forensic, and biometric applications. Besides, real-time sensing systems (based on the chemical sensors) are being researched and developed for qualitative and quantitative recognition of VOCs in body odor. The present review focuses the state-of-the-art research outcomes related to the characterization of human body odor with the objective to identify the VOCs belonging to aldehyde class. Furthermore, the application of chemical sensors in past studies for the detection of aldehydes besides other chemical compounds in body odor is summarized and the significance of aldehydes detection in different applications is discussed.

Keywords: aldehydes; characterization; chemical sensor; human body odor; VOC detection.

Introduction

Body odor is produced by skin bacteria such as Brevibacterium, Propionibacterium acnes, Corynebacterium, Staphylococcus hominis, Micrococcus luteus, and Staphylococcus epidermidis, etc. (Hart 1980, Zeng et al. 1991, Inaba and Inaba 1992, Rindisbacher 1992, Grice et al. 2009, Yamazaki et al. 2010). Skin bacteria decompose secretion outcomes (oil/wax, salts, proteins, etc.) of the sweat glands (eccrine, apocrine, etc.), which results in the complex composition of volatile organic compounds (VOCs) belonging to several chemical classes, including aldehyde, acid, amine, alcohol, hydrocarbon, ketones, sterols, sulfur compounds, and terpenoids, generating human body odor (Amoore 1977, Fang et al. 1998, Toan et al. 1999, Clancy and McVicar 2002, Jain 2004, Statheropoulos et al. 2005, Havlicek and Lenochova 2006, Steeghs et al. 2006, Wedekind et al. 2006, Penn et al. 2007, D'Amico et al. 2008b, Preti and Leyden 2010, Wisthaler and Weschler 2010, Yamazaki et al. 2010, Seeley et al. 2011, Thorn and Greenman 2012, Agapiou et al. 2015a,b, Buljubasic and Buchbauer 2015, Sorokowska et al. 2015, Allen et al. 2016, Colón-Crespo et al. 2016, Fialová et al. 2016, Gildersleeve et al. 2016, Prokop-Prigge et al. 2016, Sorokowska et al. 2016, Stefanuto and Focant 2016, Verhulst et al. 2016, Zuniga et al. 2016). Growth of bacteria living on the skin is reinforced by the secretions of body fluids from the different glands like pheromones and fatty acids (apocrine sweat glands) (Clancy and McVicar 2002, Seeley et al. 2011), ceruman (ceruminous gland) (Clancy and McVicar 2002), sebum (sebaceous glands) (Seeley et al. 2011), etc. and contributes in body odor. Human sebum is formed by UV, or O_3 induced peroxidation of unsaturated fatty acids (Osada et al. 2004, Steeghs et al. 2006, Wisthaler and Weschler 2010). The apocrine sweat glands (found in the axilla, areola, and anogenital region) have a major influence in the body odor compared to the other.

On the basis of origin, human body odor is classified into three main categories: primary, secondary, and tertiary (Amoore 1977). The primary body odor is a distinguishing attribute of an individual, which varies with age (Haze et al. 2001, Yamazaki et al. 2010, Sorokowska et al. 2015), ethnicity (Colón-Crespo et al. 2016, Prokop-Prigge et al. 2016), gender (Penn et al. 2007, Colón-Crespo et al. 2016), body parts (face, neck, breath, axilla, foot) (Gaffar et al. 1977, Yamazaki et al. 2010, Liu et al. 2013, Jha et al. 2014a, Hara et al. 2015, Fialová et al. 2016), body condition (unhealthy or healthy) (Thorn and Greenman 2012), fertility status (Gildersleeve et al. 2016), and genetic feature (Wedekind et al. 2006, Preti and Leyden 2010), etc. It has significant contribution in medical (D'Amico et al. 2008b, Buljubasic and Buchbauer 2015), security, safety and forensic (Jain 2004, Statheropoulos et al. 2005, Agapiou et al. 2015a,b, Stefanuto and Focant 2016), cosmetic (Toan et al. 1999,

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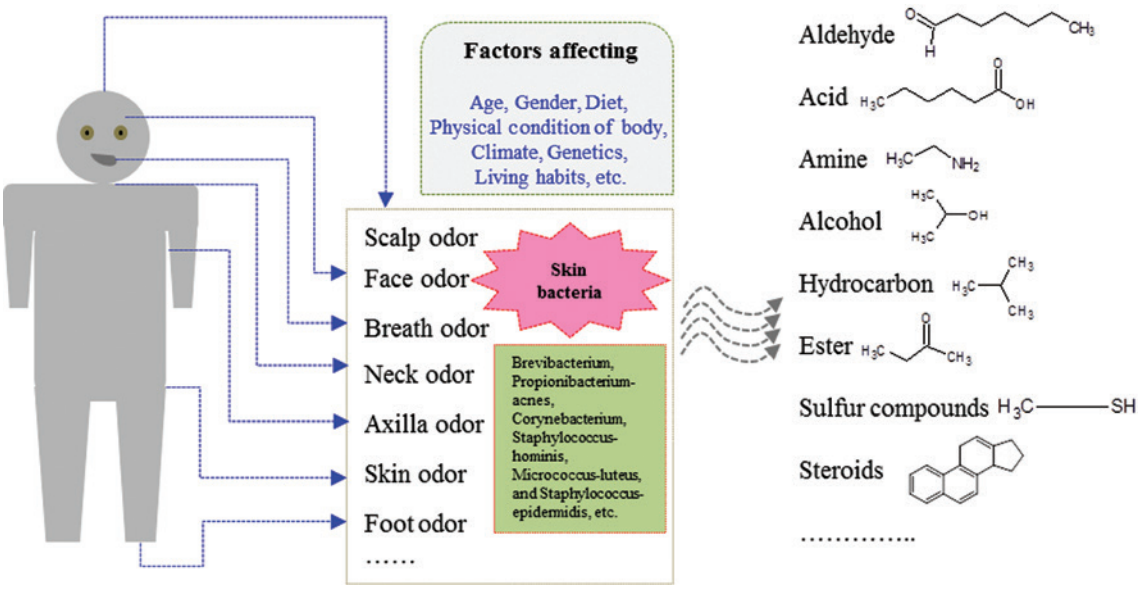

Figure 1: Schematic representation of human body odor details.

Allen et al. 2016, Sorokowska et al. 2016, Verhulst et al. 2016) applications, etc. Secondary odor is produced mainly with specific diets (meat, onion, ginger, garlic, etc.) (Havlicek and Lenochova 2006, Fialová et al. 2016, Zuniga et al. 2016), living environmental conditions (humidity, temperature, pressure, etc.) (Fang et al. 1998), etc. The usage of body soap and shampoo, perfumes, and deodorants causes a temporary, tertiary odor. The determination of the chemical composition of body odor is essential in specific applications like health monitoring, forensic investigation, biometric recognition, etc. In the beginning, canines and human sensory panels were used for the human body odor sensing. Afterward, highly sophisticated instrumental analytical methods were implemented for the qualitative and quantitative chemical composition determination of body odor. Currently, several chemical sensor-based approaches, singly or in combination with analytical methods, are in use for the real-time and fast recognition of VOCs in body odor. Past research has presented the development and future prospects of human body odor, and their related component, VOC, recognition in specific applications is summarized in some reviews (Prada and Furton 2008, Pandey and Kim 2011, Li 2014). A schematic representation of human body odor, their components, sources of origin, affecting factors, etc., is shown in the Figure 1.

Year-wise variation in the total number of published reports related to body odor research in between the years 1946 and 2015 is shown in the Figure 2 (Web of Science). It represents the superfluous research and development in last two decades.

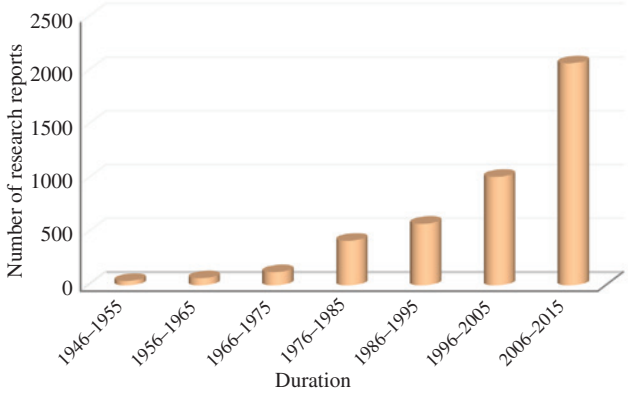

Figure 2: Published reports on body odor research (Web of Science).

Characterization of body odor

Different analytical methods have been used in the characterization of human body odor with the objective to determine the precise chemical composition of VOCs; among them, solid phase microextraction gas chromatography mass spectrometry (SPME-GC-MS) is the most common and widely used method in published literature (Zeng et al. 1991, Penn et al. 2007, Yamazaki et al. 2010, Thorn and Greenman 2012, Dormont et al. 2013b, Liu et al. 2013, Jha et al. 2014a,b, Jha and Hayashi 2015a,b, Jha et al. 2015). Besides that, GC-Fourier transform infrared spectroscopy (FTIR) (Zeng et al. 1991, Zeng et al. 1996), high-resolution GC-MS (Munk et al. 2000), thermal desorption

GC-MS (Bernier et al. 1999, Bernier et al. 2000, Penn et al. 2007), atmospheric pressure ionization (API)-MS (Martínez-Lozano and Mora 2008, Martínez-Lozano and de la Mora 2009, Martínez-Lozano 2009), GC-flame photometric detector (FPD) (Gaffar et al. 1977, Risby et al. 2001), cavity ringdown spectroscopy (CRDS) (Wang and Mbi 2007, Wang et al. 2010, Ciaffoni et al. 2012), laser spectroscopy (Mürtz 2005, Wojtas et al. 2012, Adonis et al. 2014), high-performance liquid chromatography (HPLC) (Osada et al. 2004, Ishino et al. 2010, Hara et al. 2014, Ozeki and Moro 2016), selected ion flow tube (SIFT)-MS (Enderby et al. 2009, Spanel and Smith 2011, Turner 2011), electrospray tandem-mass spectrometry (Johnson 2008), liquid chromatography-tandem mass spectrometry (LC-TMS) (Rafii et al. 2009, Lee et al. 2010), proton transfer reaction mass spectrometry (PTR-MS) (Steeghs et al. 2006, Wisthaler and Weschler 2010, Yao et al. 2015), selective reagent ionization time-of-flight mass spectrometry (SRI-TOF-MS) (Mochalski et al. 2014), and ion mobility spectrometry (IMS) (Ruzsanyi et al. 2012, Vautz et al. 2013), etc., methods have been also used in the characterization of body odor. Further details of sampling strategies, separation methods, and identification mechanisms, etc., for body odor characterization in some of the previous studies is summarized in Table 1, while characterization outcomes of odor samples from different parts of body using different analytical methods are compiled in Table 2.

Existence of aldehydes in body odor

As discussed previously, human body odor is a complex medium of various VOCs of several chemical classes. Among them, both saturated and unsaturated aldehydes were recognized as the main constituents of human body odor in many studies (Ruth 1986, Goetz et al. 1988, Kubota et al. 1994, Bernier et al. 1999, Bernier et al. 2000, Munk et al. 2000, Haze et al. 2001, Curran et al. 2005, Zhang et al. 2005, Curran et al. 2007, Penn et al. 2007, Gallagher et al. 2008, Vass et al. 2008, Hoffman et al. 2009, Vaglio et al. 2009, Ruzsanyi et al. 2012, Dormont et al. 2013a,b, Liu et al. 2013, Vautz et al. 2013, Jha et al. 2014a,b, Mochalski et al. 2014, Jha and Hayashi 2015a,b, Jha et al. 2015) in different organs, for instance, in axilla, sweat, saliva, and urine odors (Penn et al. 2007); feet odor (Dormont et al. 2013b); axilla, neck, and forehead odor (Liu et al. 2013); axilla, face, foot, neck, and forehead odor (Jha et al. 2014a,b, Jha and Hayashi 2015a,b, Jha et al. 2015); sweat/sebum odor (Munk et al. 2000); skin odor (Bernier et al. 1999, Bernier et al. 2000); skin odor (Haze et al. 2001); scalp odor (Goetz et al. 1988, Kubota et al. 1994, Zhang et al. 2005); sweat odor (Vaglio et al. 2009); skin odor (Gallagher et al. 2008); and hand odor (Curran et al. 2007) etc. Table 3 summarizes the list of aldehydes identified in the past few studies(Ruth 1986, Goetz et al. 1988, Kubota et al. 1994, Bernier et al. 1999, Bernier et al. 2000, Munk et al. 2000, Haze et al. 2001, Curran et al. 2005, Zhang et al. 2005, Curran et al. 2007, Penn et al. 2007, Gallagher et al. 2008, Vass et al. 2008, Hoffman et al. 2009, Vaglio et al. 2009, Dormont et al. 2013a,b, Liu et al. 2013, Jha et al. 2014a,b, Jha and Hayashi 2015a,b, Jha et al. 2015). A detailed analysis of human body odor (axilla, sweat, saliva, and urine) is reported by Penn et al. (2007) for determination of VOC composition in 197 subjects. A total of 373 peaks of VOCs (both individual and specific) were identified in GC-MS analysis, including four aldehydes in saliva odor. Dormont et al. (2013b) have used four sampling methods (solvent extraction, SPME [contact and headspace], and chromatoprobe dynamic headspace) in feet odor characterization, which confirms the presence of aldehydes in majority (13 out of 44 VOCs). The presence of aldehyde (peak area 5.22%) is demonstrated in GC-MS characterization of axilla, neck, and forehead odor by Liu et al. (2013). The presence of aldehydes (both as individual and common) was confirmed in face odor of four subjects by Jha et al. (2014a). In other related studies (Jha et al. 2014b, Jha and Hayashi 2015a,b, Jha et al. 2015), several branched and unbranched aldehydes were identified in the male and female axilla and foot odor, face odor (Jha et al. 2014b, Jha and Hayashi 2015a,b), and neck odor (Jha et al. 2015). Munk et al. (2000) have established the presence of aldehydes in washed clothes soiled with axilla and sebum odor. The presence of 10 aldehydes was demonstrated by Bernier et al. (1999) in skin odor (maximum relative intensity 100% for Nonanal). In another study, 17 aldehydes were identified in GC-MS analysis of skin emanations of four subjects using thermal desorption (Bernier et al. 2000).

Besides several fatty acids in breath odor, the presence of six aldehydes is also reported by Martínez-Lozano and Mora (2008). The presence of aldehydes was also confirmed in skin odor and hand odor in another study (Martínez-Lozano and de la Mora 2009) by the similar research group. Haze et al. (2001) have established the presence of six aldehydes (saturated and unsaturated) due to oxidation of fatty acids in skin odor. The presence of C_5–C_{10} and other branched aldehydes was demonstrated in hair and scalp odor by Goetz et al. (1988). In another study, Kubota et al. (1994) have also confirmed the existence of hexanal, heptanal, and decanal besides other three aldehydes. Zhang et al. (2005) have analyzed

Table 1: Experimental details of few odor characterization studies.

Reference	Analytical approach	Sampling strategy	Separation method	Identification mechanism
Zeng et al. 1991	GC-MS	Human sensory panel for olfactory sampling	Stabilwax coated column	NBS library and spectra of synthetic compounds
Penn et al. 2007		Polydimethylsiloxane (PDMS)-coated bar	DB-5MS capillary	Aligning peaks with identical spectra and elution time
Dormont et al. 2013b		Solvent extraction, SPME, chromatoprobe	ID WCOT CPSil-8CB capillary	NIST library and other published sources
Munk et al. 2000		Ranking method by human sensory panel	Capillary column	Reference compounds
Zeng et al. 1996	GC-FTIR	Human sensory panel for olfactory sampling	Stabilwax coated column	NBS library and spectra of synthetic compounds
Bernier et al. 1999, 2000	Thermal desorption GC-MS	Liquid nitrogen for cold trapping	HP5 and HP-FFAP columns	Matching the spectra of a library
Martínez-Lozano and Mora 2008, Martínez-Lozano 2009, Martínez-Lozano and de la Mora 2009	API-MS	Sampling tubes	Silica capillary	Web database mass bank
Gaffar et al. 1977	GC-FPD	Gas sampling valve	Capillary chromatographic separation	Comparing retention volume, mass spectra and calibration curve
Risby et al. 2001, Wang and Mbi 2007	CRDS	Free diffusion and typical breath collection bags	Photomultiplier tube (R74000U-09 Hamamatsu)	Change in ringdown time
Hara et al. 2014	HPLC	Auto-sampler (SIL-20 A)	Photodiode detector	Comparison of retention time
Ozeki and Moro 2016		Thermal desorption rods	Column separation	Toluene equivalent
Enderby et al. 2009	SIFT-MS	Direct sampling	Quadrupole mass spectrometer and ion counting system	SIFT-MS kinetics database
Ruzsanyi et al. 2012	IMS-GC	Cylindrical steel pot	Column separation	Comparison of retention and drift time with NIST library
Vautz et al. 2013		Sampling loop method	Column separation	Comparing mobility and retention time with ISAS database

Table 2: Summary of some body odor characterization studies.

Reference	Body odor type	Characterization method	Outcomes
Zeng et al. 1991	Axilla odor	GC-MS and GC-FTIR	C_6–C_{11} saturated and unsaturated acids as key constituents
Zeng et al. 1996		GC-FTIR	Organic acids as the characteristic VOC in both the male and female
Martínez-Lozano and Mora 2008	Breath odor	API-MS	Organic acids (C_6–C_{10}) and aldehydes as main VOCs
Gaffar et al. 1977		GC-FPD	Several VOCs of different chemical classes were established
Risby et al. 2001		GC-FPD	VOCs related to hepatic disorder
Wang and Mbi 2007		CRDS	Detection of acetone (type 1 diabetes biomarker)
Wang et al. 2010		CRDS	Discrimination of type 1 and type 2 diabetic patient and healthy subjects on basis of acetone detection
Ciaffoni et al. 2012		CRDS	Monitoring of acetone
Adonis et al. 2014		Laser spectroscopy	Acetone concentration estimation in type 1 diabetes patients
Enderby et al. 2009		SIFT-MS	Estimation of VOCs concentration in ppb level
Ligor et al. 2008		SPME-GC-MS	Identification of 38 chemical compounds
Ligor et al. 2009		SPME-GC-MS	Identification of 103 chemical compounds
Wisthaler and Weschler 2010	Skin odor	PTR-MS	Chemical compounds from carbonyl, carboxyl, groups
Steeghs et al. 2006		PTR-MS	Acetaldehyde, propanal, and other VOCS
Dormont et al. 2013b		SPME-GC-MS	44 VOCs identified in feet odor of 26 subjects
Bernier et al. 1999		Thermal desorption GC-MS	Lactic acid, aliphatic fatty acids as major VOCs
Bernier et al. 2000		Thermal desorption GC-MS	346 chemical compounds recognized effectively
Martínez-Lozano and de la Mora 2009		API-MS	Lactic acid and C_{12}–C_{18} saturated acids as significant VOCs
Hara et al. 2014		HPLC	Explanation of diacetyl metabolism
Mochalski et al. 2014		SRI-TOF-MS	Detection of aldehydes, ketones, and other VOCs
Ruzsanyi et al. 2012		IMS-GC	Detection of aldehydes, ketones, and other VOCs
Osada et al. 2004	Urine odor	HPLC	Several VOCs including 2-phenylacetamide, indole, phenol, etc.
Johnson 2008		EST-MS	Detection of genetic disorder metabolites
Rafii et al. 2009		LC-MS	Recognition of homocysteine and associated metabolites
Lee et al. 2010		LC-MS	Detection of amines
Liu et al. 2013	Sweat odor	SPME-GC-MS	Organic acids as the major chemical constituents besides other VOCs
Munk et al. 2000		High-resolution GC-MS	Esters, ketones and aldehydes as primary VOCs
Penn et al. 2007		GC-MS	Individual and gender-specific VOCs in biometric and disease diagnostic applications
Jha et al. 2014a	Face odor	SPME-GC-MS	Characteristics and common VOCs of four subjects
Jha et al. 2014b	Foot odor	SPME-GC-MS	Organic acids and aldehydes as the major chemical constituents besides other VOCs
Jha et al. 2015	Neck odor	SPME-GC-MS	Characteristics and common VOCs at different sampling time of subjects
Martínez-Lozano 2009	Hand odor	API-MS	Amines as the significant VOCs
Vautz et al. 2013	Trapped body odor	IMS-GC	Detection of aldehydes, ammonia, ketones, and other VOCs

arm skin odor and found five aldehydes besides several other VOCs. Aldehyde is also identified as a major chemical constituent in the volatile signal during the pregnancy in para-axillary and nipple-areola regions of the body (Vaglio et al. 2009). Nine aldehydes, including C_8–C_{10}, were recognized in the examination of forearm and upper back odor from 25 subjects by Gallagher et al. (2008). Sixty-three VOCs were detected in the hand odor of 60 subjects, including 14 aldehydes, by Curran et al. (2007). In another study, C_6–C_{10} and other aldehydes were detected in the axillary sweat of different subjects (Curran et al. 2005). Besides living body odor, several

Table 3: Aldehydes identified in human body odor characterization studies.

Reference	Characterization method	Odor source	Detected aldehydes	CAS no.	Quantity
Penn et al. 2007	GC-MS	Saliva odor	3,7-Dimethylocta-2,6-dienal	5392-40-5	Not available
			Undecanal	112-44-7	
			Tridecanal	10486-19-8	
			3-(4-tert-butylphenyl)-2-methylpropanal	80-54-6	
Bernier et al. 1999, 2000		Skin odor	Butanal	123-72-8	Not available
			3-Methylbutanal	590-86-3	
			2-Methylbutanal	96-17-3	
			Pentanal	110-62-3	
			Hexanal	66-25-1	
			Heptanal	111-71-7	
			Octanal	124-13-0	
			Phenylacetaldehyde	122-78-1	
			Nonanal	124-19-6	
			Decanal	112-31-2	
			Undecanal	112-44-7	
			Propanal	123-38-6	
			Nonanal	124-19-6	
			2-Methylpropanal	78-84-2	
			3,7-Dimethyl-2,6-octadienal	141-27-5	
			2-Methyl-2-butenal	497-03-0	
			Decanal	112-31-2	
			2-Methylbutanal	96-17-3	
			Dodecanal	112-54-9	
			3-Methylpentanal	15877-57-3	
			2-Methylhexadecanal	55019-46-0	
			Heptanal	111-71-7	
			Benzaldehyde	100-52-7	
			2,2-Dimethylhexanal	996-12-3	
			3-Hydroxy-4-methylbenzaldehyde	57295-30-4	
			Octanal	124-13-0	
			4-phenylmethoxybenzaldehyde	4397-53-9	
Haze et al. 2001		Skin odor	Hexanal	66-25-1	Detection rate 23–33%
			Heptanal	111-71-7	Detection rate 11–15%
			Octanal	124-13-0	Detection rate 85–89%
			Nonanal	124-19-6	Detection rate 85–89%
			Decanal	112-31-2	Detection rate 69–89%
			2-Nonenal	18829-56-6	Detection rate 0–69%
Curran et al. 2005		Axillary sweat odor	Hexanal	66-25-1	Not available
			Heptanal	111-71-7	
			Octanal	124-13-0	
			Nonanal	124-19-6	0.04–0.45 relative to decanal
			Decanal	112-31-2	Not available
			2-Furancarboxaldehyde	98-01-1	
			(E)-2-Nonenal	18829-56-6	
			Benzaldehyde	100-52-7	
			Tetradecanal	124-25-4	0.05–0.30 relative to decanal
			Undecanal	112-44-7	0.0–0.33 relative to decanal
Vass et al. 2008		Bone odor after decomposition	Decanal	112-31-2	36 ppt
			Nonanal	124-19-6	10 ppt
Dormont et al. 2013b	SPME-GC-MS	Skin odor	Hexanal	66-25-1	34–2% of total volatile compounds
			Heptenal	18829-55-5	
			Benzaldehyde	100-52-7	

Table 3 (continued)

Reference	Characterization method	Odor source	Detected aldehydes	CAS no.	Quantity
			Octenal	2548-87-0	
			Nonanal	124-19-6	
			Decanal	112-31-2	
			Undecanal	112-44-7	
			Dodecanal	112-54-9	
			Tridecanal	10486-19-8	
			3-(4-tert-Butylphenyl)-2-methylpropanal	80-54-6	
Liu et al. 2013		Sweat odor	Nonanal	124-19-6	Peak area 5.22%
Jha et al. 2014a		Face odor	Benzaldehyde	100-52-7	Peak area 7.8%
Jha et al. 2014b		Female axilla odor	Octanal	124-13-0	Peak area 8.9%
			Nonanal	124-19-6	Peak area 4.94%
Jha and Hayashi 2015a,b, Jha et al. 2015		Male and female axilla and foot odor	Hexanal	66-25-1	Peak area 1.7%
			Heptanal	111-71-7	Peak area 0.51%
			Octanal	124-13-0	Peak area 4.94%
			Nonanal	124-19-6	Peak area 5.15%
			Decanal	112-31-2	Peak area 3.87%
			Undecanal	112-44-7	Peak area 0.27%
			3-(4-tert-Butylphenyl)-2-methylpropanal	80-54-6	Peak area 0.56%
			2-Methyl-3-phenylpropanal	5445-77-2	Peak area 0.67%
			4-(1-Methylethyl) benzaldehyde	122-03-2	Peak area 0.27%
			2,3 Dihydroxy-propanal	497-09-6	Peak area 0.28%
			Tetradecanal	124-25-4	Peak area 0.20%
			2-Ethylbutanal	97-96-1	Peak area 0.13%
			2-Isopropyl-5-oxohexanal	15303-46-5	Peak area 0.20%
Zhang et al. 2005, Vaglio et al. 2009		Skin odor	Benzaldehyde	100-52-7	Not available
			Octanal	124-13-0	1.23%
			Nonanal	124-19-6	6.07%
			Decanal	112-31-2	1.23%
			3-(4-tert-Butylphenyl)-2-methylpropanal	80-54-6	Not available
			α-Hexyl-cinnamic aldehyde	101-86-0	0.270%
Curran et al. 2007		Hand odor	Hexanal	66-25-1	1.67%
			Heptanal	111-71-7	13.33%
			Benzaldehyde	100-52-7	15.0%
			Octanal	124-13-0	16.67%
			Nonanal	124-19-6	100%
			Dodecanal	112-54-9	100%
			Decanal	112-31-2	Not available
			(E)-2-Decenal	3913-81-3	
			Undecanal	112-44-7	
			Tetradecanal	124-25-4	
			(E)-2-Octenal	2548-87-0	
			(E)-2-Nonenal	18829-56-6	
			Tridecanal	10486-19-8	
			2-Methyl-2-butenal	497-03-0	
Hoffman et al. 2009		Human tissue decomposition odor	2-Hexenal	6728-26-3	Frequency 21%
			Hexanal	66-25-1	Frequency 50%
			Benzaldehyde	100-52-7	Frequency 42%
			2,4-Heptadienal	4313-03-5	Frequency 14%
			2-Heptenal	18829-55-5	Frequency 7%
			Heptanal	111-71-7	Frequency 36%
			2-Octenal	2548-87-0	Frequency 29%
			Octanal	124-13-0	Frequency 43%
			2,4-Nonadienal	5910-87-2	Frequency 14%
			2-Nonenal	18829-56-6	Frequency 29%
			Nonanal	124-19-6	Frequency 43%
			2,4-Nonadienal	5910-87-2	Frequency 21%

Table 3 (continued)

Reference	Characterization method	Odor source	Detected aldehydes	CAS no.	Quantity
Ligor et al. 2008, 2009		Breath odor	Propanal	123-38-6	<3%
			Hexanal	66-25-1	
			Heptanal	111-71-7	
			Prop-2-enal	107-02-8	Not available
			Benzaldehyde	100-52-7	Ratio 0.09–0.33
			n-Pentanal	110-62-3	Ratio 0–0.064
			Acetaldehyde	75-07-0	Ratio 0–0.071
			2-Methyl-2-propenal	19125-76-9	Ratio 0–0.035
			3-Methyl-2-butenal	107-86-8	Ratio 0–0.032
Munk et al. 2000	High-resolution GC-MS	Sweat and sebum odor in cloths	Hexanal	66-25-1	Flavor dilution (FD) factor 1, 2
			Heptenal	18829-55-5	FD 128, 512
			Octanal	124-13-0	FD 64, 512
			Octenal	2548-87-0	FD 32, 128
			(Z)-2-Nonenal	60784-31-8	FD 128, 512
			(E,Z)-2,4-Decadienal	25152-83-4	FD 1, 8
			(E,E)-2,4-Decadienal	25152-84-5	FD 16, 128
			(E)-4,5-Epoxy-(E)-2-decenal	134454-31-2	FD 16, 64
			4-Methoxybenzaldehyde	123-11-5	FD 128, 64
			2,6-(E,Z)-Nonadienal	557-48-2	FD 128
Martínez-Lozano and Mora 2008, Martínez-Lozano and de la Mora 2009	API-MS	Breath odor	3-Methylbutanal	590-86-3	Not available
			3-Methylbut-2-enal	107-86-8	
			3-Hexenal	6789-80-6	
			4-Methylpentanal	1119-16-0	
			Heptanal	111-71-7	
		Skin odor	2-Oxopropanal	78-98-8	
Goetz et al. 1988	Headspace GC-MS	Hair and scalp odor	Pentanal	110-62-3	Not available
			Hexanal	66-25-1	
			Heptanal	111-71-7	
			Octanal	124-13-0	
			Nonanal	124-19-6	
			Decanal	112-31-2	
			Undecanal	112-44-7	
			Dodecanal	112-54-9	
			Tridecanal	10486-19-8	
Kubota et al. 1994	Thermal desorption GC-MS	Hair odor	*n*-Pentanal	110-62-3	Peak area 0.53%
			Hexanal	66-25-1	Peak area 0.92%
			Heptanal	111-71-7	Peak area 0.92%
			Decanal	112-31-2	Peak area 0.92%
			Benzaldehyde	100-52-7	Peak area 0.57%
Gallagher et al. 2008	GC-MS and GC-FPD	Skin odor	Octanal	124-13-0	<2%
			Nonanal	124-19-6	<8%
			Decanal	112-31-2	<15%
			Benzaldehyde	100-52-7	Not available
			Dodecanal	112-54-9	
			2-(4-tert-Butylphenyl) propanal (*p*-tert-butyl dihydrocinnamaldehyde)	Not available	
			3-(4-tert-Butylphenyl)-2-methylpropanal	80-54-6	
			α-Hexyl cinnamaldehyde	101-86-0	
			5-(Hydroxymethyl)-2-furaldehyde	67-47-0	

aldehydes along with VOCs from other chemical classes were also identified in human body odor after decomposition (maximum frequency of occurrence 50% for hexanal among the aldehydes) by Hoffman et al. (2009). Vass et al. (2008) have also confirmed the presence of several aldehydes from buried human body decomposition.

A comprehensive list of 1870 VOCs, including several aldehydes from breath, saliva, blood, milk, skin, urine, and feces, has been reported (de Lacy Costello et al. 2014). Breath odor analysis using SPME-GC-MS by Ligor et al. (2008, 2009) recognized several aldehydes in both healthy subjects and lung cancer patients. GC-MS is a significant analytical method in human body odor characterization for the identification of chemical compounds. There are attempts to further improve the recognition performance of GC-MS method by selecting novel data sampling, increasing metabolomic exposure, and analysis methods in some recent studies (Birkemeyer et al. 2016, Delgado-Povedano et al. 2016, Jha et al. 2016).

Detection of aldehyde and other chemical compounds in body odor with chemical sensors and pattern recognition

The analytical methods were used proficiently in the characterization of human body odor for the determination of VOC composition, especially the recognition of characteristic chemical peaks related to different chemical compounds. Nevertheless, there are some practical concerns that constrain the real-time off-site applications of analytical methods, like costly, bulky, high analysis time, tough operation, etc. Therefore, the novel research focused on the development of handheld devices for instantaneous detection of VOCs present in human body odor in different applications since last few years. Especially, chemical sensor-array-based systems are established as complementary to analytical instruments in the detection of VOCs in body odor (Natale et al. 2000, Lin et al. 2001, Teo et al. 2002, Dalton et al. 2004, Vass et al. 2004, Natale et al. 2005, D'Amico et al. 2008a, Pennazza et al. 2008, Kateb et al. 2009, Wongchoosuk et al. 2009, Johnson et al. 2010, Simon 2010, Kong et al. 2011, Shirasu and Touhara 2011, Hines et al. 2012, Dymerski et al. 2013, Kybert et al. 2013, Liu et al. 2013, Jha et al. 2014b, Leunis et al. 2014, Lorwongtragool et al. 2014, Voss et al. 2014, Chinen et al. 2015, He et al. 2015, Jha and Hayashi 2015a,b, Seesaard et al. 2015, Zhao et al. 2016). However, there are a few published reports based on the detection of aldehydes in human body odor using chemical sensors. The most common types of chemical sensors used in VOC sensing applications in past studies include metal-oxide semiconductor (MOX) and conducting composite polymer (CCP) chemiresistors, quartz crystal microbalance (QCM) and surface acoustic wave (SAW) gravitational sensors, fiber-optic evanescent wave, and micro-electromechanical system sensors (Albert et al. 2000, Arshak et al. 2004, Janata 2008). Nevertheless, certain limitations of the chemical sensors, including selectivity, sensitivity, reproducibility, response time, etc., need to further improve for efficient detection of specific VOCs in the complex composition of body odor as well as in the presence of the other interfering chemicals. Previous applications of chemical sensors in human body odor sensing applications for the detection of aldehydes and other chemicals are summarized in Table 4. Other chemicals were also identified in body odor samples (Table 4), although the existence of aldehydes in previous characterization studies (Table 3) confirms the ability of chemical sensors (Table 4) in aldehyde sensing. The QCM sensor is low cost, small in size, and reliable in VOC sensing applications. The selection of suitable selective material over the surface of the QCM further improves its sensing performance. Molecular imprinted polymer (MIP) is the novel chemoselective material for the QCM sensor reported in some studies used in aldehyde sensing (Jha and Hayashi 2015a,b). Three MIPs were prepared using polyacrylic acid (PAA) as host polymer, with propenoic acid, hexanoic acid, and octanoic acid as the template molecules independently and used as chemoselective surface coating materials of four QCM sensors (three QCM coated with the MIP and one with pure PAA [non-MIP]) (Jha and Hayashi 2015a). The four-element QCM sensor array is used in the discrimination and identification of three aldehydes: hexanal, heptanal, and nonanal (established in SPME-GC-MS characterization of body odor samples) in individually as well as in binary and tertiary combinations at different concentrations (Jha and Hayashi 2015a). The best response time and recovery time for a specific MIP-QCM were 5 s and 12 s, respectively. The analysis of QCM sensor array response with principal component analysis (PCA) results in good clustering of three aldehydes and their binary and tertiary mixtures in the PC space. Support vector machine (SVM) classifier is used in quantitative class recognition (using the PC scores as input), which results in correct recognition rate of 79% for binary mixtures of three aldehydes and 83% for single, binary, and tertiary mixtures (Jha and Hayashi 2015a). In another study, novel MIPs were prepared by using PAA as host polymer and hexanal, heptanal, and nonanal as the template molecules (Jha and Hayashi 2015b). Four-element MIP-QCM sensors (three QCMs coated with the MIP and one with the non-MIP) are used for the identification of hexanal, heptanal, and nonanal

Table 4: Summary of chemical sensors used in body odor discrimination and detection of aldehydes and other chemical compounds.

Reference	Chemical sensor	Odor source	Detected aldehydes and other chemicals	CAS no.	Concentration
Jha and Hayashi 2015a,b	QCM sensor	Axilla odor, neck odor, and face odor	Hexanal Heptanal Nonanal	66-25-1 18829-55-5 124-19-6	Few parts per million (ppm)
Natale et al. 2000		Skin odor	5a-Androst-16-en-3-one	18339-16-7	Up to 50 ng/ml
Lin et al. 2001		Breath odor	Dimethylamine Trimethylamine	124-40-3 75-50-3	mg/l
Pennazza et al. 2008		Breath odor	Valeric acid Hydrogen sulphide Butyric acid	109-52-4 7783-06-4 107-92-6	Up to 2500 ppb
D'Amico et al. 2008a		Skin odor	Not available		
Vass et al. 2004	GC-MS and QCM sensor	Axilla odor	trans-3-methyl-2-hexenoic acid	27960-21-0	Not available
Teo et al. 2002	Metal oxide gas sensor	Feces, urine, saliva, and sweat odor	Not available		ml
D'Amico et al. 2008a		Axilla odor Breath odor	Isovaleric acid Not available	503-74-2	mM
Voss et al. 2014		Skin odor	Not available		
Dymerski et al. 2013		Breath odor	Chronic obstructive pulmonary disease (COPD) biomarkers		ppb
Kateb et al. 2009	CCP sensor	Glioblastoma and Melanoma cell odor	Not available		
Hines et al. 2012		Blood odor	Not available		Colony forming units (cfu)/ml
Seesaard et al. 2015		Axilla, breath, and urine odor	Not available		50–1000 ppm
Lorwongtragool et al. 2014	Carbon nanotube polymer sensor	Axilla odor	Ammonia Acetic acid Acetone Ethanol	7664-41-7 64-19-7 67-64-1 64-17-5	500 ppm
Johnson et al. 2010	Carbon nanotube field-effect transistor sensor	Breath odor	Octanal Nonanal Decanal	2548-87-0 124-19-6 112-31-2	ppm
Kybert et al. 2013		Skin odor	Nonanal	124-19-6	0.01 mg/ml
Kong et al. 2011	Chemiluminescence sensor	Proteins and cell odor	Not available		µg/ml
He et al. 2015	SAW sensor and GC-MS	Breath odor	C_6–C_{14} alkanes		ppt
Zhao et al. 2016	Optical gas sensor	Not available	Formaldehyde and other chemical compounds	50-00-0	Not available

separately and in mixtures at different concentrations. In addition, the water vapor is assumed as the significant interferents. A typical MIP-QCM sensor has a response time and recovery time of 5 s and 10 s, respectively, for one of the aldehyde odors. Better class discrimination of aldehydes was achieved in the PC space; furthermore, the SVM classifier results in 89% class recognition rate for the binary mixtures of aldehydes and 79% in the presence of single, binary, and tertiary mixtures using the PC scores (Jha and Hayashi 2015b). The medical application of VOC sensing in body odor using chemical sensors is available in some review reports (Albert et al. 2000, Arshak et al. 2004, D'Amico et al. 2008b, Janata 2008, Buljubasic and Buchbauer 2015): the past applications and future potential of chemical sensor-based artificial olfactory system (also referred as the electronic nose [E-nose]) are briefly reviewed by D'Amico et al. (2008b); applications of chemical sensors in status monitoring of diabetes by recognition of VOCs in breath, body, and urine odor are summarized by Dalton et al. (2004); Simon (2010) have presented a brief review based on cancer diagnosis by sensing the biomarker VOCs present in

human body odor with chemical sensors; a brief report based on olfactory disease diagnosis by detection of biomarker VOCs in blood, urine, breath, and skin odor is reviewed by Shirasu and Touhara (2011); and Chinen et al. (2015) have presented the significance of nanoparticle-based chemical sensing probes in the detection of cancer biomarkers. The summary of some other research reports based on human body odor and biomarker aldehyde sensing using chemical sensors is as follows. An eight-element QCM sensor array (metalloporphyrin as surface coating material) exhibits maximum efficiency in the recognition of skin odor VOCs (Natale et al. 2000). A six-element QCM sensor array was developed for uremia diagnosis by Lin et al. (2001). Sensor array response was measured for the breath odor of normal and subjects suffering from uremia, chronic renal insufficiency, and renal failure. The discriminant analysis of sensor array response results in a class recognition rate of 86.78%. The response of MOX sensor-array-based E-nose system has been measured for odors from different sources, including the sweat, urine, feces, saliva, etc., by Teo et al. (2002). The sensor array response is analyzed with the artificial neural network (ANN) in odor to discriminate the odors successfully. The human body odor decomposition database (consisting of 424 VOCs) prepared by Vass et al. (2004) is advantageous in the development of chemical sensor array portable analytical instrument for human body odor recognition. GC-MS and QCM sensor array are used in the characterization of sweat odor and recognition of present VOCs for discrimination of three groups of subjects, including those who are normal and those suffering from schizophrenia and mental disorder diseases (Natale et al. 2005). Pennazza et al. (2008) have used QCM sensor-array-based E-nose system in the detection of biomarker VOCs related to halitosis and discrimination of breath odor of normal subjects and halitosis-affected patients. Chemical sensor array has been used for discrimination between normal and malignant cells by sensing the VOCs in skin odor (D'Amico et al. 2008a). Wongchoosuk et al. (2009) have used five-element MOX sensor array (based on SnO_2 and WO_3) for human body odor (specifically the axilla odor) classification by analyzing sensor array response with the PCA. Moreover, a noise correction strategy using a humidity generator is also implemented. A 16-element CCP sensor-array-based E-nose system was developed by the Jet Propulsion Lab (JPL), USA, for the discrimination of two types of tumor cell lines by measuring the sensor response resulting from the odor of tissues (Kateb et al. 2009). A carbon nanotube field-effect transistor coated with DNA is developed for the efficient recognition of aldehydes and acids present in breath odor (Johnson et al. 2010). Nanomaterial-based chemiluminescence sensor has been developed for discrimination of normal, cancerous, and metastatic cells by using linear discriminant analysis for the response analysis by Kong et al. (2011). Cyranose 320 (32 CCP sensor array) has been used in the identification of bacteria causing ENT diseases in blood samples of patients by Hines et al. (2012). The analysis of sensor array response with the ANN methods results in a class recognition efficiency of 92.8%–97.6%. Field effect transistors using DNA-carbon-nanotube-based chemical sensor array have been used in the detection of VOCs present in skin odor. DNA-carbon nanotube functionality assists in complex body odor matrix analysis Kybert et al. (2013).

A low-cost, wearable E-nose based on CNTs/polymer sensor array is used in the identification of individual axilla odor (Lorwongtragool et al. 2014). The PCA analysis of sensor array response results in better discrimination of body odors in the PC space. A 12-element MOX sensor array (four different types in the triplicate) has been used by Leunis et al. (2014) in breath odor analysis of 23 patients suffering from head and neck cancer. The sensor array results in better discrimination of healthy and cancer-affected subjects with a sensitivity of 90% and specificity of 80%. MOX sensor-array-based E-nose is used in the discrimination of cannabis- and tobacco-consuming subjects by analyzing their skin odor (Voss et al. 2014). PCA and SVM classifier are used in the sensor array response analysis; the later results in 92.5% classification accuracy. SAW sensor and GC-MS is used in the recognition of VOCs and semi-VOCs (from parts per billion [ppb] to parts per trillion [ppt] orders) in the breath odor samples of normal subjects and cancer-affected patients (He et al. 2015). A wearable E-nose based on CCP sensors (using different polymers and carbon nanotubes) is developed and used in axilla, breath, and urine odor discrimination and recognition using PCA analysis (Seesaard et al. 2015). Metal oxide sensor array is used in the identification of 15 chronic obstructive pulmonary disease (COPD) biomarkers up to ppb levels (Dymerski et al. 2013). Optical gas sensors were used in the detection of nine gases including formaldehyde by analyzing their absorption spectra by a feature-based analysis technique (Zhao et al. 2016).

Significance of aldehyde sensing

The most significant application of aldehyde sensing in body odor is in medical diagnosis, as reported in past studies (Kateb et al. 2009, Johnson et al. 2010, Kong et al.

2011, Hines et al. 2012, Kybert et al. 2013, Lorwongtragool et al. 2014, Leunis et al. 2014, He et al. 2015, Seesaard et al. 2015), since the disease-affected body organ emits representative VOC signature, which can be used as a biomarker for diagnostic applications. Especially, characterization of axilla, skin, breath, blood, urine, etc., odor for the detection of biomarker VOCs is a significant noninvasive future medical diagnostic tool. However, there is a need to improve the selectivity and sensitivity of present chemical sensor-array-based E-nose in the recognition of disease-specific VOC in the presence of others. Quantitative detection of disease biomarker aldehydes is useful in the early presentation of diseases and progress monitoring of the patient during the treatment. E-nose could be employed as a noninvasive, real-time, precise, and fast analysis method compared to conventional disease diagnostic methods. Besides, better organization of analytical methods and E-nose could make it more effective in fast and real-time body condition monitoring. Body odor is influenced by the individual metabolic process, heredity, and living style, as mentioned earlier, which results in the distinguishable composition of VOCs. Therefore, the composition of aldehydes in body odor can be used as a biometric identification method. Body odor and mood have a convinced correlation, which can be used in the valuation of human activities like lie detection in future. The detection of VOCs in the body odor of dead people is significant in forensic applications. Also, discrimination of alive vs. dead people using VOC composition in body odor is vital for rescuing humans in natural and manmade calamities. Several aldehydes were identified in trapped body odor (Vautz et al. 2013), which could be used in forensic and rescue applications in future.

Some specific applications of aldehyde odor sensing in medical applications are as follows. 2-nominal resulting from the fatty acids is confirmed in the body odor of aged people in several studies (Haze et al. 2001, Ishino et al. 2010); consequently, it can be also used as a health biomarker. Besides nonanal, decanal and other aldehydes were also identified in skin odor, which can be used in analysis control and monitoring of skin-related diseases. The intensity of acetaldehyde and propanal in skin odor indicates the effect of UV radiation (Steeghs et al. 2006). It could be helpful in the diagnosis of skin-related diseases due to UV radiation. Controlling the concentration of nonanal and decanal was identified in foot odor (Dormont et al. 2013b) in the presence of other VOCs, which establish a possible link in origin and treatment of foot malodor. The presence of aldehydes as main odor from axilla sweat and sebum in washed and unwashed clothes (Munk et al. 2000) provides valuable information in making odor-controlling cosmetics and clothes. Detection of aldehyde plays a significant role in the diagnosis of COPD. For instance, a high concentration of malondialdehyde (propanedial) is reported in the body odor of subjects suffering from COPD (Corradi et al. 2003). Aldehydes are also established as biomarkers for other diseases like formaldehyde for breast cancer (Gordon et al. 1985), emission of acetaldehyde by malignant tissue (lung cancer cell lines) (Smith et al. 2003, Jelski and Szmitkowski 2008), etc. Several aldehydes were identified in body odor samples and originated mainly due to the lipid peroxidation of proteins (Uchida 2015); besides, butane-2, 3-dione is one of the initiators of axilla and foot odor (Hara et al. 2015).

Conclusion

The present review introduces a short description of body odor and its constituents. The analytical methods used for the characterization of human body odor with the objective to determine the composition of VOCs is briefly reviewed. The application of chemical sensor-array-based E-nose system in the detection of aldehydes in body odor and the body odor itself in several applications using some pattern recognition methods for sensors response analysis is described in detail. Lastly, the significance of chemical composition determination of body odor in different applications, especially in medical application, is highlighted. The future research in the present research domain should focus on the development of efficient body odor characterization strategy in order to search the specific biomarker VOCs in different applications. Furthermore, the development of more robust chemical sensors and pattern recognition methods for the recognition of identified VOCs in the complex matrix of body odor is also essential.

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