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Investigating the aroma of marijuana, cocaine, and heroin for forensic applications using simultaneous multidimensional gas chromatography - mass spectrometry - olfactometry

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Investigating the aroma of marijuana, cocaine, and heroin for forensic applications using simultaneous multidimensional gas chromatography- mass spectrometry – olfactometry

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DEDICATION

I would like to dedicate this thesis to my mother Feuang, my father Khouan, and my husband Ron without whose unconditional love and moral support I would not have been able to begin my educational journey. I would also like to dedicate this thesis to my children Gavin and Simon who continually show me the results of being fearless.

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ABSTRACT

The active pharmacological compound in a street drug sample is not volatile at ambient temperatures and is probably *not* what triggers and alert response from a trained drug dog. Improved understanding of the 'signature' odor characteristics of illicit street drugs offers insight into the detection and some fundamental mechanisms of canine and human olfaction. Signature odor and smell of a drug is typically caused by compounds present as very low concentrations and are not targeted in forensic analytical methods. Forensic analytical methods focus on active compounds or their breakdown intermediates, which may not elicit any olfactory response or be only a 'background' to a handful of high odor impact compounds. It has been our experience that it is typically the handful of compounds present at very low concentrations that impart the overall characteristic smell of a sample. Our working hypothesis is that a small number of volatile and semi-volatile compounds present in very low concentrations and associated with very low odor detection thresholds cause the characteristic smell of a drug. These high odor impact compounds are not being used to manufacture surrogate training scents used in training forensic canines. This omission could explain why these surrogate scents are generally not effective. This information could lead to increased understanding of what drug detection canines are using as the signature odor of street drugs. In this thesis, headspace solid phase microextraction and multidimensional gas chromatography-mass spectrometry and simultaneous olfactometry is being used for collection, separation, and identification of volatile organic compounds (VOCs) emitted from marijuana, cocaine, and heroin. Compounds with significant odor impact, as detected by human nose did not always

coincide with chemical concentration of VOCs emitted from the drug. A comparison of commercially available pseudo scent training aides versus real drug odors showed many inconsistencies. Research is warranted to continue linking smell of ‘signature’ drug aromas towards improved understanding of human and canine drug detection and olfaction.

CHAPTER 1. GENERAL INTRODUCTION

There have been landmark legal cases establishing odor as probable cause for search and seizure in the United States. See Chapter 3, SI Table 1, page 30 for a partial listing. The need for a rugged, reusable, non-invasive, non-destructive sampling device in forensic science is crucial to maintaining the integrity of evidence samples. Solid phase microextraction (SPME) allows criminalists to sample volatile organic compounds (VOCs), and in the case of this study, extract the compounds responsible for odor of marijuana, cocaine, and heroin. SPME is ideal for forensic applications due to its portability, allowing for onsite sampling and ease of transport to the lab for analysis.

SPME

85 µm Stableflex Carboxen/Polydimethylsiloxane (PDMS), 24 gauge SPME fibers were used in this study. The porous Carboxen coating retains small analytes in its pores. Carboxen/PDMS also extracts by adsorption, because it is a liquid phase coating. Another advantage of using PDMS phases for SPME analysis of VOC is its similarity to their use as gas chromatography (GC) phases[1]. The SPME fiber is essentially an inside-out GC capillary analytical column.

There are many steps in SPME method development. These steps include optimization of extraction mode, agitation considerations, and optimal sample volume, determination of extraction time, and finally calibration and validation of methods[1]. Due to the nature of the samples used in this study (illegal drugs), only extraction time and to some extent, sample volume, was open for exploration. Carboxen/Polydimethylsiloxane (PDMS) fiber coating was chosen for its wide range of selectivity for odorous volatiles.

For this reason, extraction times of 5 min, 1 h, and 68 h were used. For comparison to surrogate scents, 1 h extraction time was used for experiments with marijuana, cocaine, heroin, and their respective surrogate scents. A mini review of research using SPME for forensic applications can be found on page 31.

Multidimensional gas chromatography – mass spectrometry – olfactometry (MDGC-MS-O)

MDGC-MS-O analytical instrumentation was used in this study. The multidimensional gas chromatography comes from the setup of the analytical capillary columns; a non-polar pre-column and a polar analytical column are connected in series. This allows for separation due to boiling points, first on the pre-column, then further separation due to interactions with the stationary phase of the analytical column. This helps to tease out VOCs that may be co-eluting and allows for better resolution between peaks, two common problems with odor analysis. The novelty of this instrumentation stems from the way data generated by olfactometry with a human panelist are collected simultaneously with data generated by allows the researcher to assign an odor character, hedonic tone, and intensity to a chemical compound. A mini review of instrumentation used for analysis of volatiles from illicit drugs can be found on page 31.

Volatile organic compounds emitted from illegal drugs

Research has been done to identify the VOCs present in headspace of illegal drugs; details of this are further outlined in the individual chapter introductions to follow. This research highlights three important cases to consider when characterizing the odor of drugs: 1) chemicals detected by MS have an odor, 2) chemicals detected by MS *do not* have an odor, and 3) chemicals with trace or no detection by MS have a definite odor. The assumption that big chemical peaks equate big odor impact has been proven

incorrect [2, 3] and the shift to using odor detection thresholds (ODTs) to quantify forensic odor is warranted.

Research Motivation

(1) This thesis applies the concept of odor activity value (OAV) to offer one explanation as to propose a new way to calculate the “characteristic” odor of any forensic sample. This can be done without a state of the art MDGC-MS-O.

(2) This thesis also investigates why commercial surrogate scent formulations do not smell like their drug counterparts, as seen by field tests with drug detection dogs [4, 5]. Better understanding of the target odor will lead to better formulations of surrogate scents for training purposes.

Thesis Organization

Chapters 2 and 3 are modified from a manuscript submitted *to Forensic Science International* on March 31, 2015. Specifically, these two chapters correspond to the first research goal of using OAV to quantify odor character. Chapters 4 and 5 are modified from a second manuscript submitted to the same journal on June 12, 2015. These last two chapters correspond to the second research goal of using OAVs to explain why current surrogate drug scent formulations do not smell like the real drugs they are meant to mimic.

References

1 Pawliszyn, J. *Solid Phase Microextraction: Theory and Practice. (Wiley-VCH, 1997) p 97-139.*

2 Lo, Y.-C. M. *et al.* Simultaneous chemical and sensory characterization of volatile organic compounds and semi-volatile organic compounds emitted from swine manure using solid phase microextraction and multidimensional gas chromatography-mass spectrometry-olfactometry. *Journal of Environmental Quality* **37**, 521-534, doi:10.2134/jeq2006.0382 (2008).

3 Vance, E. Profile: What is that smell? *Nature* **455**, 726-728 (2008).

4 Lorenzo, N. *et al.* Laboratory and field experiments used to identify Canis lupus var. familiaris active odor signature chemicals from drugs, explosives, and humans. *Analytical and Bioanalytical Chemistry* **376**, 1212-1224, doi:10.1007/s00216-003-2018-7 (2003).

5 Macias, M. S., Harper, R. J. & Furton, K. G. A comparison of real versus simulated contraband VOCs for reliable detector dog training utilizing SPME-GC-MS. *American Biotechnology Laboratory* **26**, 26-27 (2008).

CHAPTER 2. CHARACTERIZING THE SMELL OF MARIJUANA BY ODOR IMPACT OF VOLATLE COMPOUNDS. AN APPLICATION OF SIMULTANEOUS CHEMICAL AND SENSORY ANALYSIS.

Modified from a paper submitted to *Forensic Science International*

Somchai Rice [a, b], Jacek A. Koziel [b, *]

Abstract

Recent US legislation has permitted recreational use of marijuana in certain states. The use of marijuana odor as probable cause for search and seizure is brought to the forefront of forensic science. This study shows the use of solid-phase microextraction with multidimensional gas chromatography – mass spectrometry and simultaneous human olfaction to characterize the total aroma of marijuana. The application of odor activity analysis offers an explanation as to why high volatile chemical concentration does not equate to most potent odor impact. This suggests that more attention should be focused on highly odorous compounds typically present in low concentrations, such as nonanal, decanol, o-cymene, benzaldehyde, which have more potent odor impact than previously reported marijuana headspace volatiles.

Introduction

Americans know the Fourth Amendment of the U.S. Constitution protects citizens from unreasonable search and seizure, without a warrant, by government bodies. Landmark legal cases have set a precedent of what is deemed probable cause. A review of legal cases can be found on page 30. Courts are challenged to be consistent with using odor of marijuana as probable cause when recreational use is now legal in some states and illegal at the federal level. Thus, the scent, its chemistry and

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environmental fate affects a whole set of issues beyond scent detection and recognition. Previous research has been conducted on the volatile organic compounds (VOC) present in the headspace of marijuana. The major components of total VOC in headspace of the plant material has been reported to consist of limonene[1-5], α-pinene[1,3,4,6], β-pinene[1,3,4,6], β-myrcene[1,3-5], β-ocimene[2,4], β-caryophyllene[2,4-6], α-caryophyllene[4,6], α-phellandrene[4], 3-carene[4], α -terpinene[4], terpinolene[4], terpineol[5], linalool[4,5], α-cadinene[4]. To date, a total of approximately 31 compounds are known to be emitted from marijuana[1-6].

The smell of marijuana has been investigated using dogs[7-9] and humans[10]. Different options are available for canine scent training tools[11-13], even a marijuana odor mimicking incense[14]. There is a reported method for concealing marijuana odor[15]. It is impossible to determine causes an alert response from canines, simply because dogs cannot tell us. Limited work has been published on canine and human detection of marijuana odor, yielding mixed results and high variability. A review of research on canine and human olfaction of marijuana odor is given on page 32. A thorough, analytical approach to the investigation of marijuana odor detected by humans is warranted, if and when more states seek to legalize recreational use.

The objectives of this study were to (1) identify odorous compounds emitted from marijuana using multidimensional gas chromatography tandem mass spectrometry coupled with simultaneous *human olfaction* and (2) show an application and novelty of odor activity values (OAV) to better understand the ‘characteristic’ aromas of marijuana (3) explore aromatic compounds that are emitted through packaging typical in illicit distribution of marijuana. The working hypothesis is that simultaneous chemical and

sensory analysis can elucidate the identity of aromatic compounds that are responsible for the characteristic smell of marijuana. This information is needed to (a) better understand which compounds are really responsible for the “characteristic” aroma of marijuana, (b) provide additional insight into aroma perception by applying a method (i.e., OAV) established in food and beverage field in a new setting (i.e., forensic sciences), and (c) investigate how marijuana packaged for illicit distribution can smell differently according to these odor activity values.

With improved analytical techniques, the list of identified compounds is increasing, starting from 20 compounds in 1973[1] with an addition of 10 new compounds since[1-6]. Even though more compounds have been identified, it has not increased understanding of forensic *odor*.

1. Odor activity value

A caveat is offered for equating high chemical concentration to high odor impact. Odor perception is much more complicated and this laboratory has illustrated this phenomenon, highlighting the role of highly odorous compounds present at extremely low concentrations[16]. There are two big hurdles when using GC for characterization of odorous compounds: sufficient resolution between the compounds, and co-elution of two or more of these compounds. A GC using a non-polar column connected in series to a polar analytical column can account for such occurrences[17,18]. The use of state-of-the-art *simultaneous* multidimensional-GC-MS-olfactometry (MDGC-MS-O) allows researchers to separate, at high resolution, odors that may not be separated on a single column, and to detect compounds[18] based on their odor activity values (OAV). This report is the first instance of using MDGC-MS-O to characterize the odor of marijuana.

Since the introduction of GC-O, intensity and odor character of an individual compound has been better described[19]. Patton and Josephson originally presented the concept of the OAV[20].

$$OAV = [Concentration]/ODT \quad \textbf{(Eq. 1)}$$

where ODT is odor detection threshold and defined as the concentration a compound is detected by 50% of the population

OAV has been used extensively in the food and beverage industry to characterize aroma of bread, beef, coffee, beer [21] and wines [22,23] and more recently odor emissions from animal buildings [24]. This report is the first application of OAV to characterize marijuana. This paradigm shift from concentration based (i.e., high concentration, potent odor) to OAV based aroma detection of marijuana and associated odor perception can help extend the knowledge of marijuana odor and its role in forensic science.

Materials and Methods

The marijuana samples were obtained from Iowa Division of Criminal Investigation (Iowa DCI), Drug Identification Section. Marijuana was available in various states of seizure and included: 1) a US military-style duffel bag filled with marijuana weighing ~ 50 kg; 2) 1 gram air-dried marijuana (*loose*); 3) 1 gram of the same air-dried marijuana placed in a plastic zip-top sandwich bag (*bagged*).

Carboxen/Polydimethylsiloxane (PDMS), 85 µm Stableflex, 24 gauge solid-phase microextraction (SPME) fibers were used (Sigma-Aldrich, St. Louis, MO, USA). Briefly, experimental conditions were as follows: the drugs were placed in separate, pre-

cleaned and baked 16 ounce mason jars with modified lids. The Carboxen/PDMS fibers were exposed to the headspace and volatiles were collected; equilibration time was the same as extraction time. Headspace-SPME extraction was carried out at 5 min, 1 h, and 68 h at ambient temperature. When the extraction step was completed, the SPME fiber was retracted, wrapped in pre-baked aluminum foil, placed in a pre-cleaned mason jar, and transported back to the laboratory in a cooler on ice. In the laboratory, fibers loaded with VOC were stored in a 4 °C refrigerator until analysis, wrapped in the foil and sealed in a clean mason jar. SPME fibers were exposed to the heated injection port of the MDGC-MS-O for thermal desorption and analysis. Please see SI Figure 1 and SI Figure 2 for additional information.

MDGC-MS-O analysis was performed on an Agilent 6890 GC, with a restrictor guard column, non-polar capillary column (BP-5, 56 m x 530 µm inner diameter x 1.00 µm thickness, SGE, Austin, TX, USA) and polar capillary column (BP-20, 25 m x 530 µm inner diameter x 1.00 µm thickness, SGE, Austin, TX, USA) connected in series. Outflow from analytical column was held at 7.0 cc/min. Sample flow was split 3:1 via open split interface to the sniff port and mass spectrometer, respectively, as determined by restrictor column inner diameter. Desorption time was 2 minutes in splitless mode at 270 °C under flow of helium carrier gas (99.995% purity). Subsequent analysis of the same fiber immediately afterward, revealed no carry over. The oven temperature was programmed as follows: 40 °C for 3.00 minutes, then increased to 220 °C at a rate of 7.00 °C per minute, and held for 11.29 minutes (40 minutes total run time). The carrier gas was set at constant pressure at the midpoint (junction point of the non-polar and polar column) at 5.8 psi. Transfer line to the MS was set at 240 °C; transfer line to the

sniff port was set at 240 °C with humidified air set at 8.00 psi. MS heated zones were 150 °C for the quadrupole and 230 °C for the source. Mass spectrometer parameters were electron impact (EI), electron energy set to 70eV, and acquisition range m/z 33.0-280.0 u.

The instrument was tuned daily and column blanks were performed and did not show any contaminating compounds. Analysis of blank trip fiber (an unloaded SPME fiber taken to the site and back, stored with fibers to be analyzed) at the end did not show any contaminating compounds. VOCs were identified tentatively using the Automatic Mass Spectral Deconvolution and Identification System (AMDIS) and six specialty mass spectral libraries derived from the NIST05/EPA/NIH mass spectral database. It was not appropriate to use retention indexes (Kovats RI) for identification due to the configuration of the capillary columns, but known retention times of standards previously analyzed on this system were also used for identification.

There were four parameters recorded for perception of odorants during olfactometry work outlined in this study. First parameter was detectability, defined here as the minimum concentration of the odorant needed to be recognized. Published odor detection threshold values are not fixed numbers, but are set to represent the concentration that 50% of the population can detect [25]. Intensity for each aroma note was also recorded, and defined here as the perceived strength of the aroma event. Guidelines for intensity scale were used as follows: not present = 0, faint = 25, distinct = 50, strong = 75, intense = 100. The character, or aroma descriptor, describes what the odor smells to the trained panelist. A descriptor of “characteristic” was used when an odor was distinguished to represent the overall aroma of the sample. Hedonic tone was

the user-defined parameter of pleasantness or unpleasantness. In this study, a nine-level classification scale was used. This range was from -4 (a very unpleasant odor) through 0 (a neutral odor) up to +4 (a very pleasant odor). Area under the peak of each aroma event in the aromagram is calculated as Aroma Area = Width x Intensity x 100, where width is the length of time in min that an aroma persisted.

Results and discussion

In this study, a total of 233 compounds were tentatively identified as volatiles in headspace emitted from marijuana at room temperature (Table 1). This list was compiled from analysis of lab-stored, desiccated marijuana (SI Figure 1) and newly seized, fresh marijuana (SI Figure 2), in packed and unpackaged form. Over 200 new compounds were added to the list of volatiles known to be emitted from marijuana. Newly reported compounds, represent an addition of 95% of the total compounds reported in Table 1.

1. Permeation of marijuana volatiles through packaging

Exploration of the effects of packaging and dwell time of marijuana in packaging (i.e. sampling time and storage/equilibrium time in the package were identical) revealed an increase in the number of chromatographic peaks detected, with increased headspace sampling time, in both the loose and bagged marijuana. Figure 1 shows an overlay of the total ion chromatogram (TIC) generated by the MS showcasing detected VOCs emitted from loose marijuana in a sealed glass jar and detected VOCs emitted *through* a plastic zip-top sandwich bag in a sealed glass jar.

Across all 3 sampling times, 134 total volatiles were identified from headspace emitted from marijuana, through a plastic zip-top sandwich bag (page 34) and loose (page 47) with a net match of 65% or higher from AMDIS (National Institute of Standards and Technology, Gaithersburg, MD). Data analysis using all 6 specialty libraries provided in AMDIS resulted in 20, 54, and 101 chromatographic peaks identified in the loose marijuana and 25, 39 and 108 chromatographic peaks identified in the bagged for sampling times of 5 min, 1 h, and 68 h, respectively. Previously reported volatiles (bolded in Table 1) are known to elute between 6 min and 22 min on the MDGC-MS-O system used in this study (see Figure 1). Please see SI Table 2 and SI Table 3 for full details regarding the identification, odor character, and odor activity values of these 134 compounds. Results indicate that the number of unique VOC present in headspace of marijuana increase with time, stored at room temperature, and with or without packaging.

The effect of packaging on concentration of VOCs (seen as relative peak area counts of a mass selective detector) of the 134 total VOCs emitted marijuana was not statistically significant ($p > 0.05$). There was statistically significant effect of sampling time on concentration (seen as relative peak area counts) for 34% of the VOC emitted from marijuana ($p < 0.05$). See SI Table 4 for full summary of F-statistics and p-values from statistical analysis. Compounds previously reported as key components of marijuana odor (α-humulene[4,6] and β- caryophyllene[2,4-6]) did not permeate through packaging after 5 min. β- Caryophyllene[2,4-6] did not permeate through packaging after 1 h. After 68 h of storage, 51 of 53 total compounds permeated through plastic packaging. Preliminary results show that packaging of marijuana in plastic zip-top

sandwich bags does not have a significant effect on VOC emitted (i.e. odorous VOC), but storage time has a significant effect on the concentration of VOC emitted (i.e. more time allowed for more odorous VOC to be emitted). Specifically, by 68 h, the concentrations of volatiles emitted were significantly higher than at 5 min, regardless of packaging. Marijuana recently stored in a plastic sandwich bag (i.e. 5 min) will have a different odor profile than marijuana stored in a plastic bag for 68 h.

Table 1. Comparison of (a) 233 volatiles found in this study emitted from marijuana, including those emitted through-packaging with (b) volatiles previously reported as 'signature' compounds of marijuana in headspace

This Study (a)	(-)-Aristolene	(-)-Globulol	(+)-4-Carene	(+)-calarene	(+)-nerolidol
	(+)-sativene	(1R)-(+)-trans-isolimonene	1-(3-methylphenyl)-ethanone	1-(3-methylphenyl)-ethanone	1,1-dimethyl-hydrazine
	1,2,3,4-tetramethylbenzene	1,2-diethylbenzene	1,3,5-triazine-2,4,6-triamine	1,3-dichlorobenzene	1,4-diethylbenzene
	1-butanol	1-butoxy-2-propanol	1-hexadecanol	1-hexanol	1-undecanol
	2,2,5-trimethylhexane	2,3,4-trimethylpentane	2,4,6-trimethylphenol	2,4-di-tert-butylphenol	2,6-diethylpyrazine
	2,6-dimethylquinoline	2-butanone	2-butoxyethanol	2-chloroacetophenone	2-ethenyl-1,3-dimethylbenzene
	2-ethoxyethanol	2-ethylhexanol	2-ethyltoluene	2-heptanone	2-hydroxyacetophenone
	2-isopropenyl-3-methylpyrazine	2-methyl naphthalene	2-methyl-1H-imidazole	2-methyl-2-propanamine	2-methylaziridine
	2-methylpentane	2-nitropropane	2-phenoxyethanol	3,4,5-trimethyl-1-hexene	3,4,5-trimethylphenol
	3-ethyl-o-xylene	3-ethyltoluene	3-isopropylbenzaldehyde	3-methyl-2-cyclopenten-1-one	3-methylheptane
	3-methylpentane	3-pentanol	4-ethoxy-3-anisaldehyde	4-methyl guaiacol	4-methyldecane
	4-methylphenethylamine	4-methylpyrimidine	4-pyridinamine	5-ethenyl-2-methylpyridine	5-methylindane
	5-octanolide	7-methoxycoumarin	Acetaldehyde	Acetamide	Acetic acid
	Acetone	Acetophenone	Acrolein	Alloaromadendrene	Anethole
	Aromadendrene	Benzaldehyde	Benzonitrile	Benzophenone	Benzphentamine
	Benzyl acetate	Benzyl Alcohol	Benzyl formate	Benzyl nitrile	Betahistine
	Betazole	Butane	Butyl formate	**Camphene**	Carbofuran
	Carvacrol	**Caryophyllene oxide**	Cedryl acetate	cis-2-pinanol	Citronellolformate
	Citronellyl acetate	Cumene	Cuminaldehyde	Decanal	Diacetone alcohol
	Dibutyl phthalate	Diethyl Phthalate	Dimethylbenzylcarbinyl acetate	Dimethylpyrazine	Dimethylsulfide
	Dimethylsulfone	DL-carvone	Dodecane	Durene	Dyclocaine
	Estragole	Ethanol	Ethylacetate	Ethylene oxide	Ethylenediamine
	Ethylenimine	Eugenol	Eugenyl acetate	**Fenchyl alcohol**	Formic acid
	Furfural	Furfurylmethylamphetamine	Heptanal	Hexadecane	Hexanal
	Hexanoic acid, methyl ester	Hexanoic acid, propyl ester	Hexestrol	Hordenine	Hydrazine
	Isoamyl alcohol	Isobornyl acetate	Isobornyl thiocyanoacetate	Isobutane	Isobutyraldehyde
	Isobutyrophenone	Isocyanatomethane	Isodurene	Isoeugenol	Isoprene
	Isoquinoline	**Limonene**	Limonene dioxide	**Linalool**	Linalyl acetate
	Longifolene	m-cymene	Methacrolein	Methacrylic anhydride	Methyl acetate
	Methyl acetylsalicylate	Methyl anthranilate	Methyl benzoate	Methyl heptadienone	Methyl heptanoate
	Methyl isoeugenol	Methyl mercaptan	Methyl salicylate	Methyl valerate	Methylene chloride
	methylhydrazine	Methylisohexenyl ketone	m-tert-butylphenol	Myrcene	Nerol
	Nerolidol	Nitrobenzene	Nonanal	Nonane	Octanal
	o-cymene	o-dimethyl hydroquinone	o-guaiacol	o-methylacetophenone	o-xylene

Bolded compounds indicate concurrent identification with this study and previously reported studies. Underlined compounds indicate compounds previously reported but not found in this study. No true "blank" package sample type was available for comparison of the same material and manufacturing lot of the seized illicit marijuana. Therefore, this report is conveying all compounds found in headspace of marijuana, regardless of packaging type and presence.

Table 1 continued

	p-acetanisole	p-aminotoluene	**p-cymene**	Pentadecane	Pentamethylbenzene
	Pentanal	Perillaldehyde	p-ethyltoluene	Phenol	Phenylethyl alcohol
	Piperidine	Piperonal	p-methylacetophenone	Propanal	Propanoic acid, anhydride
	Propofol	Propylamine	Propylene glycol	p-tert-butylphenol	p-xylene
	Sabinene	Salicyladehyde	Styrene	**Terpinolene**	tert-butanol
	tert-butyl-benzene	Tetrahydrozoline	Thymol	Toluene	Tridecane
	Tyramine	Undecane	**Valencene**	Verbenone	α-bisabolol
	α-bulnescene	**α-cadinene**	α-cedrene	α-copaene	α-cubebene
	α-guaiene	α-gurjunene	**α-humulene**	α-ionol	α-longipinene
	α-methylcinnamaldehyde	**α-phellandrene**	**α-pinene**	**α-terpinene**	α-terpineol
	β-caryophyllene	β-cedrene	β-irone	**β-pinene**	**β-selinene**
	γ-gurjunene	γ-hexalactone	**γ-terpinene**	**δ-3-carene**	δ-cadinene
	3-(1-methylethyl)-phenol methylcarbamate		3-methyl-5-(1-methylethyl)-Phenol methylcarbamate		
	3-(3-hydroxyphenyl)-2-propenoic acid, methyl ester		1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide		
Previously reported (b)					
Porto (2014)[4]	(E)-ocimene	**Limonene**	**Linalool**	**Terpinolene**	**α-cadinene**
	α-humulene	**α-phellandrene**	**α-pinene**	**α-terpinene**	**β-caryophyllene**
	β-myrcene	**β-pinene**	**δ-3-carene**		
Rather (2011)[6]	1,8-Cineole	3-Hexen-1-ol-acetate	**Camphene**	Cis-Hex-3-en-1-ol	Eudesma-3,7(11)- diene
	Guaiol	**Limonene**	**Valencene**	**α-humulene**	**α-pinene**
	β-caryophyllene	β-chamigrene	β-maaliene	β-ocimene	**β-pinene**
	β-selinene				
Lai (2008)[2,3]	**Limonene**	**α-pinene**	**β-caryophyllene**	β-myrcene	β-ocimene
	β-pinene				
Osman (1985)[5]	**β-caryophyllene**				
Hood (1973)[1]	**Camphene**	**Caryophyllene oxide**	**Fenchyl alcohol**	**Limonene**	**Linalool**
	Methyl heptenone	p-**cymene**	**Terpinolene**	α-Bergamotene	**α-humulene**
	α-pinene	**α-terpinene**	**β-caryophyllene**	β-Farnesene	β-myrcene
	β-ocimene	β-phellandrene	**β-pinene**	**γ-terpinene**	**δ-3-carene**

Bolded compounds indicate concurrent identification with this study and previously reported studies. Underlined compounds indicate compounds previously reported but not found in this study. No true "blank" package sample type was available for comparison of the same material and manufacturing lot of the seized illicit marijuana. Therefore, this report is conveying all compounds found in headspace of marijuana, regardless of packaging type and presence.

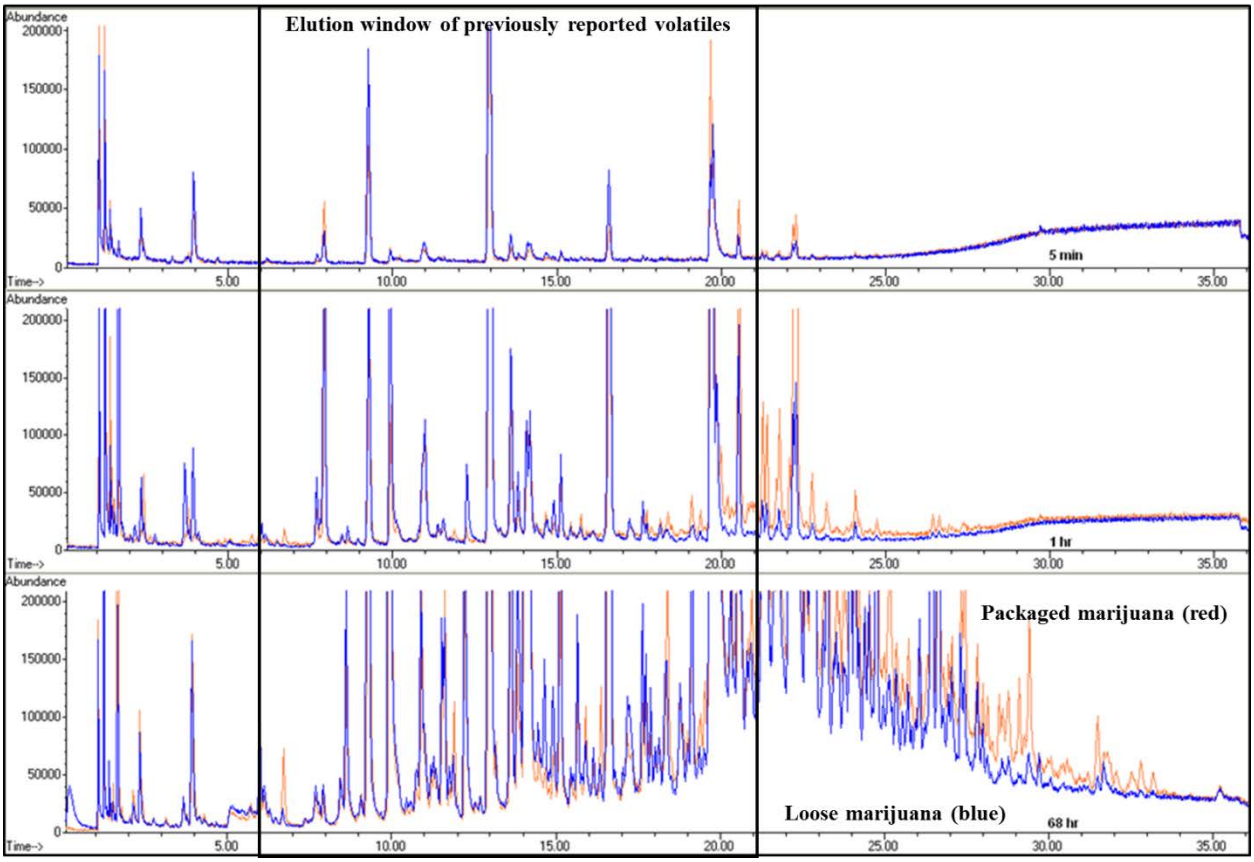

Figure 1. Effects of equilibration time/sampling time on HS-SPME of marijuana, loose in a sealed glass jar and bagged in plastic zip-top sandwich bag and sealed in a glass jar. From top to bottom, the set of 3 TIC represent 5 min, 1 h, and 68 h extraction/sampling time resulting in 20, 54, and 101 chromatographic peaks (blue), and 25, 39, 108 chromatographic peaks (red), respectively, at room temperature using 85 µm Carboxen/PDMS SPME fiber. Vertical axis is scaled to equal detector response. The boxed retention time widow highlights where volatiles, from previously published articles, would elute from the analytical column of the MDGC-MS. See SI Table 2 and for the complete summary of identified compounds.

2. Application of OAV to marijuana volatiles

There were 124 chemical peaks tentatively identified using MDGC-MS, thought to be compounds emitted from marijuana through plastic zip-top sandwich bag regardless of sampling time (SI Table 2). Only 8% of the compounds detected by MS had published odor descriptors (19% and 58% for 1 h and 68 h, respectively). Eight %

had published odor detection thresholds (11% and 41% for 1 h and 68 h, respectively). A total of 121 chemical peaks were tentatively identified by MDGC-MS directly emitted from marijuana (a.k.a., loose) regardless of sampling time (SI Table 3). Only 9% had published odor descriptors (31% and 59% for 1 h and 68 h, respectively). Seven % had published odor detection thresholds (20% and 38% for 1 h and 68 h, respectively). These numbers show that researchers only know as much as 59% of the information in terms of odor description, and 41% of the information in terms of odor detection threshold. Further research to reveal this missing information is warranted.

A Wilcoxon signed rank test of paired samples was performed (SI Table 5) for each combination of time and packaging. This test compared the number of times when concentration is greater than calculated OAV, to the number of times when calculated OAV is greater than concentration, taking into account the size difference within the pairs. The null hypothesis is there is no difference in number of oppositions in each direction. Results indicated there is a significant difference between concentration and calculated OAV (using (Eq. **1** and listed in SI Table 2 and SI Table 3) for loose marijuana at 1 h and 68 h extraction ($p = 0.014$ and $p < 0.0001$, respectively) and marijuana in a plastic zip-top bag at 68 h extraction ($p < 0.0001$) . See page 64 for statistical details of Wilcoxon signed rank test for all possible combinations. VOC were ranked by concentration (smallest concentration = 1) for bagged marijuana, shown in SI Table 6. This illustrates how high chemical abundance does not correspond to high odor intensity as perceived by human nose. Most importantly, compounds that have previously been reported as important volatile markers of marijuana based on high concentration and found in this study actually rank lower when using OAV (SI Figure 3**,**

SI Figure 4**,** SI Figure 5) and vice versa. In other words, concentration of VOC and calculated OAV are not highly correlated ($R^2 < 0.638$; See SI Table 7). A general trend, based on available published human odor detection threshold, is that less concentrated compounds could have more impact on odor, and therefore should be more responsible for the overall characteristic odor than the most concentrated compounds.

3. Simultaneous chemical and sensory analysis of fresh marijuana

There were 179 compounds identified by MDGC-MS using AMDIS and 53 odor events associated with simultaneous olfactometry during a 68 h extraction of volatiles emitted from fresh marijuana through a cloth duffel bag (SI Figure 2). Only 29% of the chemicals present in headspace of this marijuana sample registered an odor response by human nose. Only 31% of the 179 compounds had published odor detection thresholds in order to calculate odor activity value. Using Flavornet[26] and The Good Scents Company (TGSC)[27] aroma databases, 62% of the 179 compounds had a description of aroma perceived by human nose. Sensory data presented in this study only represent about 30% of the total amount of compounds detected by MS, due to unknown or unplublished odor detection thresholds and the subsequent calculation of OAV ((Eq. **1**). See SI Table 8 for full details of all 179 compounds and 53 aroma events, associated aromas, odor detection thresholds and calculated odor activity for volatiles emitted from fresh evidence marijuana and emitted through a cloth duffel bag over 68 h.

A comparison of the total ion chromatogram generated by MS and aromagram generated by human olfaction is shown in Figure 2, illustrating simultaneous chemical and sensory detection of extracted volatiles in headspace emitted through a duffel bag.

- **Case A** (black-outlined box) illustrates the current understanding of compounds responsible for aroma of marijuana, showing a large chemical signal with a large olfactory intensity. There were 20 instances (9% of the identified peaks) of Case A.
- **Case B** (black-outlined box) illustrates where a chemical present in the headspace has no perceived aroma by human nose. There were 159 instances (75% of identified peaks) of Case B.
- **Case C** (black-outlined box) illustrates the paradigm shift of odor perception that is the main focus of this report. Chemicals having small concentration (i.e. sub-threshold detection by mass spectrometer), can register high odor impact due to odor activity value (Eq. 1). There were 34 instances (16%) of Case C.

Note the 5 “characteristic” aromas detected by human nose, with the exception of Case A (identified by AMDIS as β-pinene), were not the most chemically abundant in headspace, and perceived to represent the overall aroma of marijuana. Equilibrium of volatiles and semi-volatiles in the sample, the headspace of the closed sampling system, and the fiber coating was assumed after 68 h. Full identification and odor characteristics of volatiles belonging to these 3 cases are shown in SI Table 8. This suggests that compounds having very small concentration in headspace of marijuana are the “needles in the haystack” of compounds responsible for overall odor of marijuana, *not* the most concentrated compounds as previously reported.

There were 53 aroma events identified by human panelist (Table 2) found in the fresh marijuana sample in a duffel bag, emitted over 68 h (SI Figure 2). The overall hedonic tone of the sample can be described as 71% unpleasant, 5% pleasant and 22% neutral. Aroma event 36 was rated the most intense but with relatively small chemical

signal from the mass detector, described as moldy, burnt, and burnt food by the panelist. The 5 “characteristic” aromas had intensities of 80, 80, 70, 60, and 60. The aroma events were ranked by aroma area (assumed to be equivalent to mass detector response); the “characteristic” aromas are within the top 15 most intense aromas. When these volatiles were ordered by concentration and compared to the odor activity values, we observed the same trend in rank shift (Figure 3), also observed in SI Figure 3, SI Figure 4, and SI Figure 5 indicating that concentration and odor impact are not highly correlated ($R^2 < 0.1047$, SI Table 7).

Figure 3 shows 79 compounds with published ODT, emitted from all marijuana samples presented thus far. It is pointed out that because of missing published ODT for some compounds, this ranking by OAV only shows information representing less than 47% of the total compounds detected by MS. Only 56 out of 178 volatiles emitted from marijuana through a cloth duffel bag, over 68 h, have published ODTs. More research is warranted to establish these missing ODTs. Shown in Figure 3, 3.7% of these 79 compounds were unique to dry marijuana in a plastic zip-top sandwich bag, 2.4% were unique to loose, dry marijuana, 34.5% were unique to fresh marijuana in a duffel bag. Highlighted in Figure 3 is α-pinene, ranked 49th (high) in concentration in headspace of fresh marijuana emitted through a duffel bag, but is ranked 25th (low to mid-range) in odor activity value. Nerol is ranked 6th (low) in concentration in headspace of fresh marijuana emitted through duffel bag, but is ranked 51st (high) in odor activity value. Current research misses the target when only the highly concentrated compounds

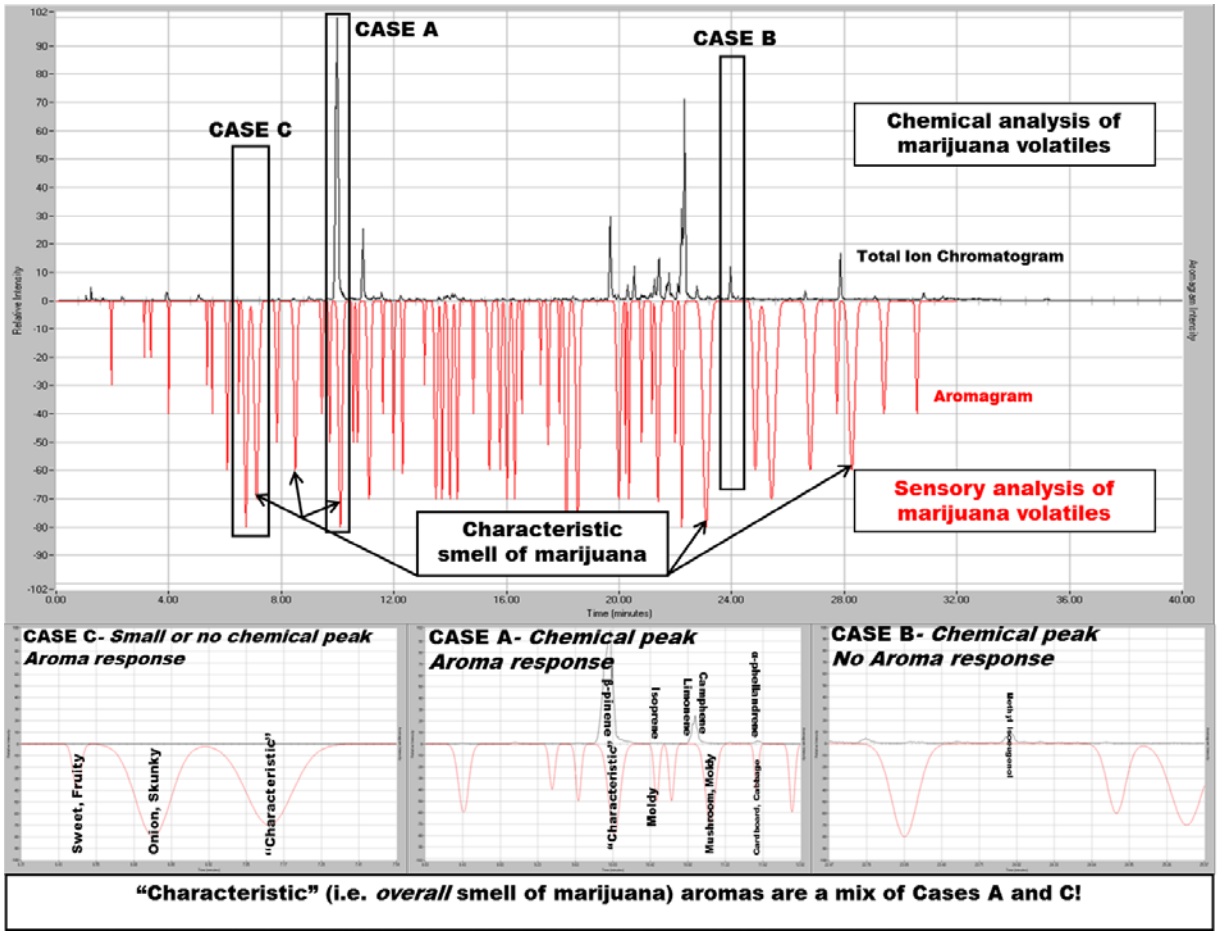

Figure 2. Overlay of simultaneous chemical and sensory analysis of volatiles emitted into headspace, through a duffel bag and captured by SPME over 68 h. Total ion chromatogram (TIC), black, and Aromagram, red and inverted, of VOCs emitted from marijuana in a duffel bag. An 85 µm Carboxen/PDMS SPME fiber was exposed to HS over the duffel bag, within an overturned glass jar to capture emitted volatiles for 68 hours. A total of 53 aroma events (Table 2) and 178 compounds were recorded (SI Table 8). Aroma events # 12, 15, 46, and 51 were recorded as a "characteristic" smell (i.e. the aromas that most represent the overall aroma of marijuana). Outlined cases signify (A) big chemical peak detected, smell detected; (B) chemical peak detected, no smell detected; (C) Small or no chemical peak detected, smell detected. Zoomed Case A, B, and C boxes show identification of chemical peaks and aromas detected.

Table 2. Aroma profile of volatiles emitted through a duffel bag and collected on SPME over 68 h generated by human panelist.

Event#	RT (min)	Descriptor	Hedonic Tone	Width (min)	Intensity	Aroma Area
1	1.92	Plastic, Solvent	Unpleasant -1	0.09	30	269
2	3.09	Onion, Garlic	Unpleasant -1	0.08	20	159
3	3.31	Moldy	Neutral 0	0.11	20	219
4	3.96	Sweet, Solvent	Neutral 0	0.08	40	319
5	5.32	Cardboard	Unpleasant -1	0.08	30	239
6	5.50	Sweet, Fruity	Pleasant +2	0.08	40	319
7	6.00	Grassy, Aldehydic	Neutral 0	0.18	60	1078
8	6.46	Sweet, Fruity	Pleasant +2	0.07	40	279
9	6.59	Onion, Skunky	Unpleasant -3	0.32	80	2555
10	6.92	Resiny, **Characteristic**, Onion, Skunky	Unpleasant -3	0.42	70	2935
11	7.74	Smoky, Resiny, Potato	Unpleasant -1	0.21	50	1048
12	8.36	Resiny, Potato, **Characteristic**	Unpleasant -1	0.3	60	1797
13	9.36	Medicinal, Herbaceous	Unpleasant -2	0.16	40	638
14	9.64	Herbaceous, Medicinal	Unpleasant -2	0.16	50	798
15	9.93	Aldehydic, Citrus, Mint, **Characteristic**	Unpleasant -3	0.34	80	2715
16	10.48	Moldy	Unpleasant -1	0.14	50	698
17	10.64	Onion, Garlic, Skunky, Medicinal	Unpleasant -3	0.15	50	748
18	10.98	Mushroom, Moldy	Neutral 0	0.29	70	2026
19	11.55	Cardboard, Cabbage	Neutral 0	0.12	40	479
20	11.91	Onion, Garlic, Skunky, Sulfury	Unpleasant -3	0.16	60	958
21	12.23	Acidic, Burnt, Fatty Acid	Unpleasant -3	0.17	61	1035
22	13.04	Moldy, Burnt	Unpleasant -1	0.12	30	359
23	13.37	Moldy, Burnt, Burnt food	Unpleasant -3	0.25	70	1747
24	13.63	Potato, Resiny, Roasted	Unpleasant -2	0.18	70	1257
25	13.86	Roasted, Potato, Resiny, Moldy	Unpleasant -1	0.27	70	1886
26	14.15	Burnt, Burnt food	Unpleasant -3	0.21	70	1467
27	14.78	Mushroom, Moldy	Neutral 0	0.1	40	399
28	15.28	Moldy, Burnt, Burnt food, Fatty acid	Unpleasant -3	0.23	60	1377
29	15.68	Herbaceous, Spicy, Burnt food, Fatty acid, Burnt	Unpleasant -4	0.19	60	1138
30	15.90	Medicinal, Herbaceous	Unpleasant -4	0.24	70	1677
31	16.18	Soapy, Citrus, Mint	Neutral 0	0.22	70	1537
32	16.50	Herbaceous, Medicinal	Unpleasant -2	0.11	40	439
33	17.16	Skunky, Sewer	Unpleasant -2	0.11	30	329
34	17.40	Moldy, Burnt food	Unpleasant -2	0.17	51	865
35	17.82	Citrus, Herbaceous	Neutral 0	0.12	40	479
36	18.01	Moldy, Burnt food, Burnt	Unpleasant -4	0.26	90	2336
37	18.37	Herbaceous, Medicinal	Unpleasant -3	0.34	80	2715
38	19.83	Burnt food, Burnt, Piggy, Urinous	Unpleasant -3	0.34	70	2376
39	20.20	Herbaceous, Smoky	Unpleasant -2	0.07	61	426
40	20.29	Herbaceous, Citrus	Neutral 0	0.14	70	978
41	20.73	Herbaceous, Citrus, Resiny	Unpleasant -1	0.15	50	748
42	21.12	Moldy	Neutral 0	0.11	40	439
43	21.24	Sweet, Fruity	Pleasant +2	0.28	71	1984
44	21.91	Herbaceous, Resiny	Unpleasant -1	0.16	50	798
45	22.13	Gasoline, Solvent	Unpleasant -3	0.21	80	1677
46	22.79	Herbaceous, Resiny, Medicinal, **Characteristic**, Piggy, Urinous	Unpleasant -3	0.6	80	4792
47	24.64	Medicinal, Herbaceous, Resiny	Unpleasant -3	0.42	60	2515
48	25.07	Piggy, Urinous, Barnyard	Unpleasant -4	0.72	70	5031
49	26.53	Piggy, Barnyard, Urinous	Unpleasant -3	0.54	60	3234

Event number is the order of elution from the chromatography column. Retention time (RT). Intensity (scale of 0 to 100, 100 is most intense). Aroma Area = Width x Intensity x 100.

Table 2 continued

Event#	RT (min)	Descriptor	Hedonic Tone	Width (min)	Intensity	Aroma Area
50	27.63	Potato, Resiny	Unpleasant -1	0.23	40	918
51	27.98	Resiny, Potato, Roasted, **Characteristic**	Unpleasant -1	0.58	60	3474
52	29.22	Potato, Resiny	Neutral 0	0.38	40	1517
53	30.47	Potato, Resiny	Neutral 0	0.23	40	918

Event number is the order of elution from the chromatography column. Retention time (RT). Intensity (scale of 0 to 100, 100 is most intense). Aroma Area = Width x Intensity x 100.

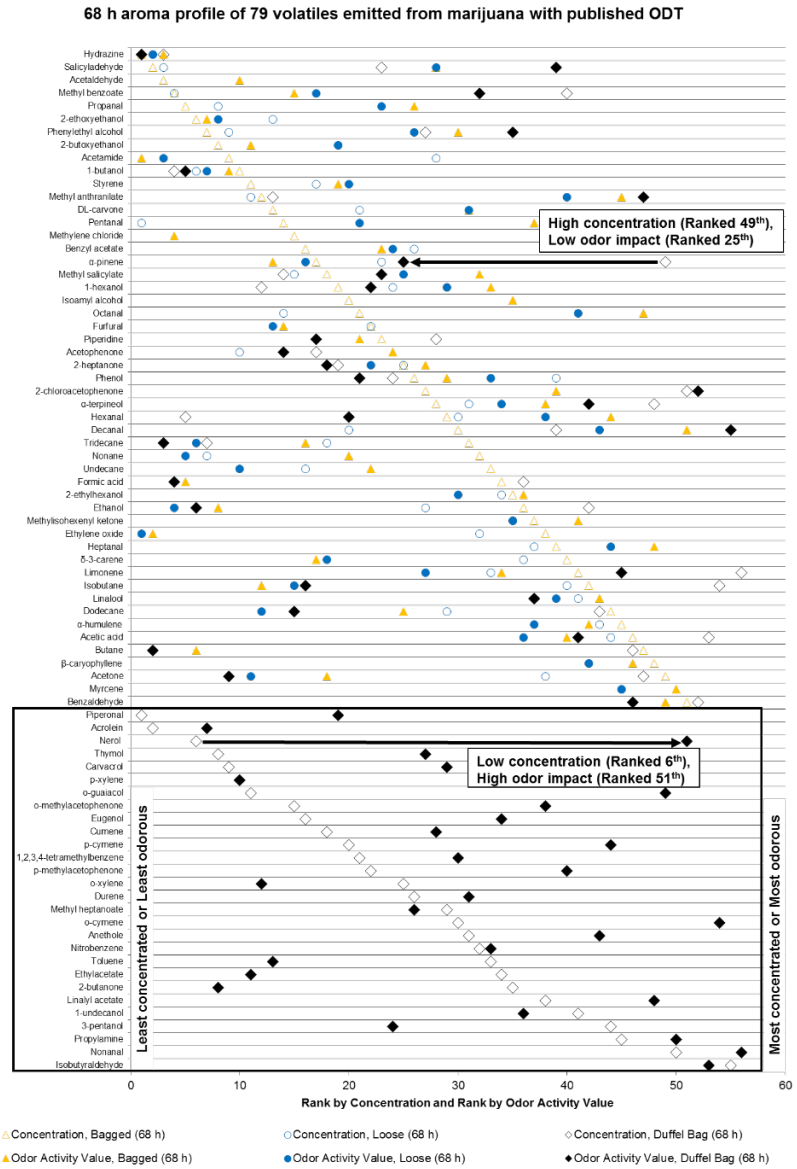

Figure 3 .Dot plot illustrating hierarchy of volatiles emitted from marijuana over 68 h at room temperature in terms of concentration and calculated OAV from published ODT. Compounds are ranked by concentration (△, ◊, ○), and calculated OAV (▲, ♦, ●). Data representing bagged (in plastic zip-top sandwich bag) and loose marijuana sampled for 68 h are imported from SI Figure 5. Rank value (on horizontal axis) of 1 indicates low concentration or low OAV; rank of 56 indicates high concentration or high OAV. The general trend is a shift in rank based on odor activity value (e.g., marijuana in a duffel bag (◊, ♦), Nerol has a rank of 6 by concentration and has a rank of 51 by aroma impact (OAV); α-pinene has a rank of 49 by concentration and has a rank of 25 by aroma impact (as OAV). Calculation of OAV is shown in (Eq. 1. Values of rank for each VOC are given in SI Table 6. The black-boxed compounds highlight VOC that were detected in fresh marijuana and *permeated* through a duffel bag, not detected or permeated in desiccated marijuana.

are investigated when trying to understand odor. These data also suggest that the complete odor profile of fresh marijuana emitted through a duffel bag is caused by a mix of compounds different from dry marijuana (*loose*) or dry marijuana in a plastic zip-top sandwich bag.

Figure 4 illustrates that the most odorous compounds with published ODT found to be responsible for the overall aroma of dry marijuana investigated in this research, both *loose* and *emitted through a plastic zip-top bag* over 68 h are 1) Benzaldehyde, 2) Myrcene, 3) Decanal, 4) Heptanal, 5) Methyl anthranilate, 6) Octanal, 7) Hexanal, 8) Methylisohexenyl ketone, 9) Linalool, 10) β-Caryophyllene, 11) α-Humulene, and 12) Acetic acid. Highly odorous compounds with published ODT emitted from fresh marijuana *through a duffel bag* over 68 h are A) Nonanal, B) Decanol, C) o-Cymene, D) Isobutyraldehyde, E) 1-Chloroacetophenone, F) Nerol, G) Propylamine, H) o-Guaiacol, I) Linalyl acetate, J) Methyl anthranilate, K) Benzaldehyde, L) Limonene. The top ranked volatile compounds (by odor activity values) are not identical to those currently known as key odorous compounds responsible for the smell of marijuana. Also, results of this research indicate the key odorous compounds responsible for the smell of marijuana are different between old, desiccated marijuana and fresh marijuana.

4. *Odor impact based on OAV*

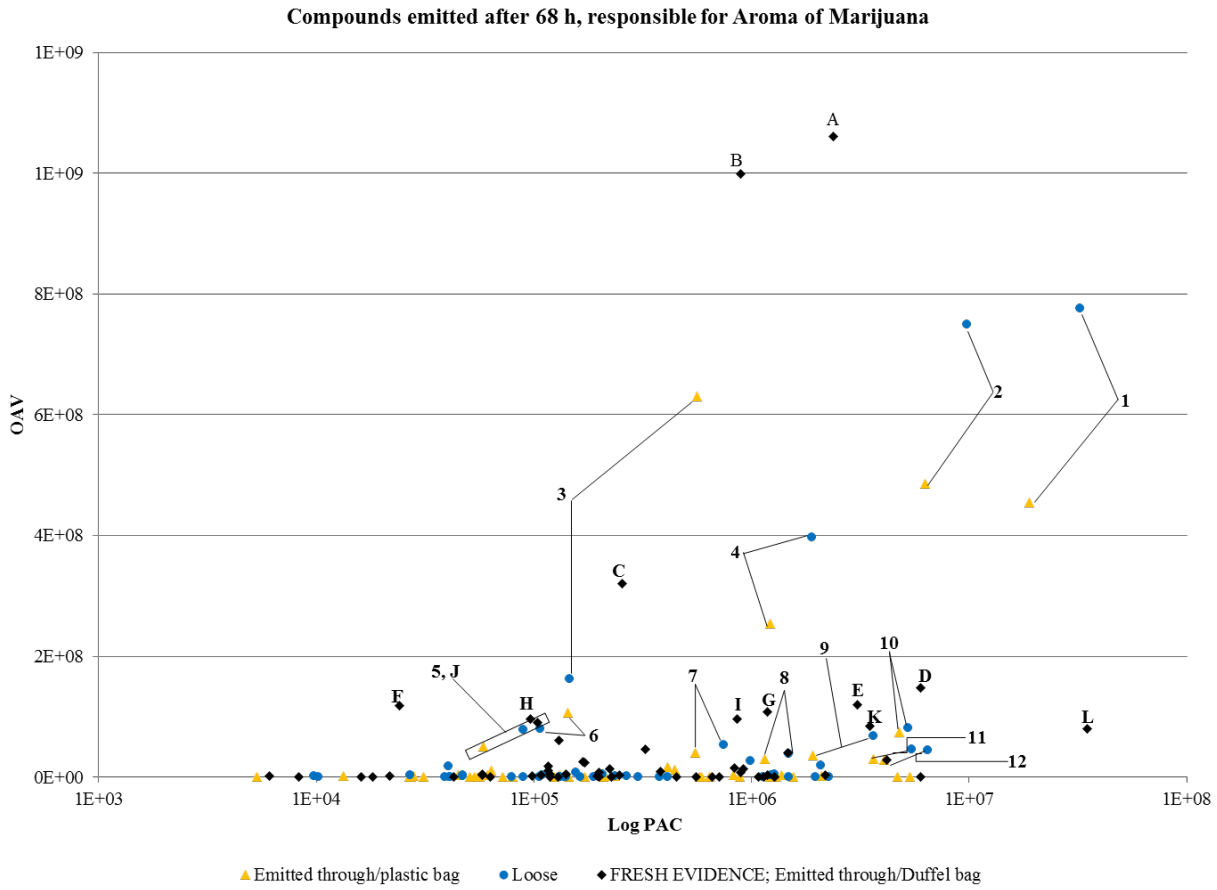

Figure 4. Compounds with high odor impact are not always the most abundant in concentration. Horizontal axis is peak area counts (PAC) of mass detector response, assuming equal response for all compounds. Vertical axis is calculated OAV (Eq. 1) for each compound. Highly odorous compounds emitted from *loose* marijuana (blue circles) and *through packaging* (yellow triangles) over 68 h at room temperature are 1) Benzaldehyde, 2) Myrcene, 3) Decanal, 4) Heptanal, 5) Methyl anthranilate, 6) Octanal, 7) Hexanal, 8) Methylisohexenyl ketone, 9) Linalool, 10) β-caryophyllene, 11) α-humulene, 12) Acetic acid. Highly odorous compounds emitted from fresh evidence of marijuana *through a duffel bag* (black circles) over 68 h at room temperature are A) Nonanal, B) Decanol, C) o-cymene, D) Isobutyraldehyde, E) 1-chloroacetophenone, F) Nerol, G) Propylamine, H) o-guaiacol, I) Linalyl acetate, J) Methyl anthranilate, K) Benzaldehyde, L) Limonene

Conclusions

Odorous compounds emitted from marijuana were identified using multidimensional GC-MS coupled with simultaneous *human olfaction*. Over 200 compounds are being

added to the list of what is currently known to be emitted from illicitly packaged marijuana. It is suggested that newly packaged marijuana (i.e. packaged or sitting in a room for 5 min) would have a different aroma profile than marijuana that has been stored for a longer period (i.e. packaged or sitting in a room for 68 h) due to the increased number of chemical peaks detected by MDGCMS-O (~20 compounds to ~100 compounds, respectively). Overall odor of marijuana due to compounds emitted is time dependent, but effects of plastic zip-top sandwich bag or cloth duffel bag packaging on compound concentration were not significant ($p < 0.05$). When simultaneous chemical and sensory analysis was used to analyze headspace volatiles of marijuana emitted through a duffel bag, 9% of the chemicals detected by MS had an associated aroma, 75% of the chemicals detected did not have an aroma detected, and 16% registered low or no chemical signal but an aroma was detected. This phenomenon can be explained by taking into account OAVs. To date, application of odor activity values to forensic odor is a novel approach. More work is needed to establish ~55% of missing odor detection thresholds and ~41% missing odor description. This reports suggests that highly odorous compounds are not necessarily the most concentrated compounds in headspace. This is the first reported instance of using multidimensional GC-MS tandem *simultaneous* olfactometry by human nose to characterize the volatiles in the total aroma profile emitted from marijuana in the context of non-destructive, through-packaging analysis of evidence. This draws attention to how training a drug detection dog, handlers, and other law enforcement officers to a handful of compounds does not cover the gamut of VOC found in different conditions of marijuana for illegal distribution.

References

1 Hood, L. V. S., Dames, M. E. & Barry, G. T. Headspace volatiles of marihuana. *Nature* **242**, 402-403, doi:10.1038/242402a0 (1973).

2 Lai, H., Corbin, I. & Almirall, J. R. Headspace sampling and detection of cocaine, MDMA, and marijuana via volatile markers in the presence of potential interferences by solid phase microextraction-ion mobility spectrometry (SPME-IMS). *Analytical and Bioanalytical Chemistry* **392**, 105-113, doi:10.1007/s00216-008-2229-z (2008).

3 Lai, H., Guerra, P., Joshi, M. & Almirall, J. R. Analysis of volatile components of drugs and explosives by solid phase microextraction-ion mobility spectrometry. *Journal of Separation Science* **31**, 402-412, doi:10.1002/jssc.200700292 (2008).

4 Porto, C. d., Decorti, D., Natolino, A. & da Porto, C. Ultrasound-assisted extraction of volatile compounds from industrial Cannabis sativa L. inflorescences. *International Journal of Applied Research in Natural Products* **7**, 8-14 (2014).

5 Osman, A. & Caddy, B. Analysis of cannabis using tenax-GC. *Journal of the Forensic Science Society* **25**, 377-384, doi:10.1016/s0015-7368(85)72417-6 (1985).

6 Rather, M. A. *et al.* Headspace solid phase microextraction (HS SPME) gas chromatography mass spectrometric analysis of the volatile constituents of Cannabis sativa L. from Kashmir. *Journal of Pharmacy Research* **4**, 2651-2653 (2011).

7 Lorenzo, N. *et al.* Laboratory and field experiments used to identify Canis lupus var. familiaris active odor signature chemicals from drugs, explosives, and humans. *Analytical and Bioanalytical Chemistry* **376**, 1212-1224, doi:10.1007/s00216-003-2018-7 (2003).

8 Macias, M. S., Harper, R. J. & Furton, K. G. A comparison of real versus simulated contraband VOCs for reliable detector dog training utilizing SPME-GC-MS. *American Biotechnology Laboratory* **26**, 26-27 (2008).

9 Jezierski, T. *et al.* Efficacy of drug detection by fully-trained police dogs varies by breed, training level, type of drug and search environment. *Forensic Science International* **237**, 112-118, doi:10.1016/j.forsciint.2014.01.013 (2014).

10 Doty, R. L., Wudarski, T., Marshall, D. A. & Hastings, L. Marijuana odor perception: Studies modeled from probable cause cases. *Law and Human Behavior* **28**, 223-233, doi:10.1023/B:LAHU.0000022324.13389.ea (2004).

11 Curtis, P. E. & Arden, G. A. Odor recognition training system for training dog to recognize desired odor to detect e.g. cocaine for indoor/outdoor applications, has reward release system operated by trainer for dispensing reward directly from storage compartment. US8776731-B1.

12 Curry, W. Animal trainer e.g. for training dog to recognize an object e.g. ball or package with a distinctive odor, e.g. marijuana, has solenoid which is operatively connected to movable plunger barrier for allowing ball to move. US6571743-B1.

13 Curry, W. Remote control ball ejector. US 6571743 (2003).

14 Martin, K. E. Incense producing scent like marijuana|contg. ground alfalfa, bay leaves and starch binder. US4158549-A.

15 Elrod, S. Method for using scent elimination device to conceal contraband e.g. marijuana, involves generating gaseous stream of descenting material containing ozone, and dispersing descenting material over contraband to eliminate scent. US2010071633-A1; WO2010065103-A1; US8187533-B2.

16 Cai, L., Koziel, J. A. & O'Neal, M. E. Determination of characteristic odorants from Harmonia axyridis beetles using in vivo solid-phase microextraction and multidimensional gas chromatography-mass spectrometry-olfactometry. *Journal of Chromatography A* **1147**, 66-78, doi:10.1016/j.chroma.2007.02.044 (2007).

17 Lo, Y.-C. M. *et al.* Simultaneous chemical and sensory characterization of volatile organic compounds and semi-volatile organic compounds emitted from swine manure using solid phase microextraction and multidimensional gas chromatography-mass spectrometry-olfactometry. *Journal of Environmental Quality* **37**, 521-534, doi:10.2134/jeq2006.0382 (2008).

18 Vance, E. Profile: What is that smell? *Nature* **455**, 726-728 (2008).

19 Marin, A. B., Acree, T. E., Hotchkiss, J. H. & Nagy, S. Gas – chromatography olfactometry of orange juice to assess the effects of plastic polymers on aroma character. *Journal of Agricultural and Food Chemistry* **40**, 650-654, doi:10.1021/jf00016a026 (1992).

20 Patton, S., and D.V. Josephson. A method for determining significance of volatile flavor compounds in foods. *Food Res.* **22**, 316-318 (1957).

21 Grosch, W. Determination of potent odourants in foods by aroma extract dilution analysis (AEDA) and calculation of odour activity values (OAVs). *Flavour and Fragrance Journal* **9**, 147-158, doi:10.1002/ffj.2730090403 (1994).

22 Guth, H. Quantitation and sensory studies of character impact odorants of different white wine varieties. *Journal of Agricultural and Food Chemistry* **45**, 3027-3032, doi:10.1021/jf970280a (1997).

23 Ferreira, V., Ortin, N., Escudero, A., Lopez, R. & Cacho, J. Chemical characterization of the aroma of Grenache rose wines: Aroma extract dilution analysis, quantitative determination, and sensory reconstitution studies. *Journal of Agricultural and Food Chemistry* **50**, 4048-4054, doi:10.1021/jf0115645 (2002).

24 Parker, D. B. *et al.* Odor and odorous chemical emissions from animal buildings: Part 6. odor activity value. *Transactions of the Asabe* **55**, 2357-2368 (2012).

25 *Odor Thresholds for Chemicals with Established Occupational Health Standards*. 90 (AIHA, 1989).

26 Acree, T. E. & Arn, H. *Flavornet and human odor space*, http://flavornet.org/flavornet.html (2004). Accessed August 8, 2014.

27 The Good Scents Company Information System, http://www.thegoodscentscompany.com/index.html# (1994). Accessed September 8, 2014.

CHAPTER 3. CHARACTERIZING THE SMELL OF MARIJUANA BY ODOR IMPACT OF VOLATLE COMPOUNDS. AN APPLICATION OF SIMULTANEOUS CHEMICAL AND SENSORY ANALYSIS (Supporting Information)

Modified from a paper submitted to *Forensic Science International*

Somchai Rice [a, b], Jacek A. Koziel [b, *]

SI Table 1. Legal cases based on probable cause for search and seizure.

Legal Case	Ruling
Payton v. New York (1980)[1]	A warrantless search **inside your home** is reasonable if there is *probable cause* or exigent circumstances
Maryland v. Macon (1985)[2]	A warrantless search **inside your home** is reasonable if items are in plain view
Davis v. United States (1946)[3]	A warrantless search **inside your home** is reasonable if an officer is given consent
United States v. Robinson (1973)[4]	A warrantless search **inside your home** is reasonable if the search is incident to a lawful arrest
New Jersey v. TLO (1985)[5]	A warrantless search of **a student** under the authority of school officials is reasonable
Arizona v. Gant (2009)[6]	A **vehicle** may be searched in the area where evidence might be found, if there is *probable cause* of the vehicle containing evidence of criminal activity
Illinois v. Cabales (2005)[7]	A narcotics detection dog may walk around the exterior of the **vehicle** in a valid traffic stop without reasonable or explainable suspicion
United States of America v. Harris (1994)[8]	Police officers used the smell of marijuana as *probable* cause to search a **vehicle** only to find cocaine in the car, but no marijuana.

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Review of research using SPME for forensic applications

Solid phase microextraction (SPME) was used as a non-destructive, non-invasive, sampling device to collect volatiles permeated through packaging and responsible for 'characteristic' aroma of marijuana. The use of micro-sampling techniques in forensic science has been reviewed in Kabir (2013)[9]. SPME is favored due to a smaller requirement on sample size, eliminated use of organic solvents, portability, and lends itself to automation[9]. SPME is also best at reducing matrix effects inherent in forensic work with blood, plasma, and urine[10]. Headspace (HS) sampling using SPME for characterization of volatile organic compounds (VOC) has been used to characterize explosives[11], confiscated 3, 4-methylenedioxy-N-methylamphetamine (MDMA a.k.a. Ecstasy) and amphetamine[12], cocaine[13]. The upsurge in the use of SPME for all-in-one sample preparation, cleanup, and pre-concentration of volatiles in forensics highlights its importance to the field.

Review of instrumentation used for analysis of volatiles from illicit drugs

There are some clear favorites in instrumentation being used for analysis of headspace VOC emitted from marijuana. Gas-chromatography (GC) was used to distinguish marijuana of different geographic origins, with unsuccessful results for classification[14]. GC tandem mass-spectrometry (MS) was used to characterize volatile oil composition of dried and fresh marijuana buds[15], and to discern differences between volatile compounds found in male and female marijuana plants of Northern Lights and Hawaiian Indica[16]. Volatile composition of entire inflorescences of hemp have been analyzed by GC-MS[17], even with ultrasound-assisted extraction[18].

Review of research in canine and human olfaction of marijuana odor

Dogs trained for specific odor detection (e.g. narcotics, explosives, cadavers) are the current benchmark used in the law enforcement community. A study by Macias *et al.* in 2008[19] showed that a mixture of α-pinene, β-pinene, myrcene, limonene, and β-caryophyllene associated with marijuana showed low alert responses when field tested on narcotic detection dogs. None of the dogs alerted to Sigma Pseudo Marijuana scent[19] (Sigma Aldrich, St. Louis, MO, USA). In a separate study comparing dogs trained and tested with illicit drugs, (i.e., 68 Labrador retrievers, 61 German shepherds, 25 terriers and 10 English cocker spaniels), it was found that German shepherds were superior scent dogs and terriers were inferior at detecting drugs. The researchers tested 5 types of illicit drugs and found that marijuana was the easiest for all dogs to detect, followed by hashish, amphetamine, cocaine, and lastly heroin. In over 1000 trials, the dogs found the hidden drugs within 64 sec and an 87.7% accuracy rate (5.3% false positive)[20]. It has also been shown that the dog handler may also affect alert responses, with a failure rate of 85% false positives during search of a clean room[21]. With such a large range of variability, research is warranted to discover what triggers an alert from the dogs.

In a situational based study by Dotty in 2004, subjects were asked to smell a garbage bag containing 5 pounds of marijuana, and a garbage bag of crushed newspapers[22]. All human subjects could identify the bag containing marijuana. Could these same people detect marijuana smell sitting in the driver's compartment, with the marijuana in a garbage bag inside the car trunk? False positives (9.36%) was the same as true positives (12.97%), with $p > 0.20$, meaning there was no significant difference in

detecting the marijuana bag versus the newspaper bag. Next, the researchers wanted to know if budding and non-budding marijuana plants produce similar odors (i.e. mature versus non-mature plants, respectively). A tomato plant was used as the negative control. All participants found mature (budding) plant volatiles more intense ($p < 0.025$) suggesting the buds hold the odorous compounds. Odor intensities of immature cannabis did not differ significantly from the tomato plant. Lastly, the researchers wanted to test if the smell of marijuana can be distinguished when it is mixed with diesel exhaust. The rates of detection when combined with diesel exhaust were not significant[22].

SI Table 2. Summary of VOCs emitted from marijuana though packaging into headspace and captured by SPME during 5 min, 1h, 68 h static sampling at room temperature.

							Published Descriptors		Published ODT (ppm)			
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
Ethylene oxide	75-21-8	5 min	1	1.06	4: 44 45 132 46	66				8.51E+02	1.42E+06	1.66E+03
		68 h	1	1.07	2: 44 45	66				8.51E+02	1.22E+06	1.43E+03
2-nitropropane	79-46-9	5 min	2	1.12	2: 43 58	72				7.24E+00	1.24E+04	1.71E+03
		1 h	1	1.12	2: 41 43	75				7.24E+00	6.30E+03	8.69E+02
Isobutane	75-28-5	1 h	2	1.23	10: 43 42 41 39 72 55 50 73 71 58	84				1.00E+01	7.18E+06	7.18E+05
		68 h	2	1.24	6: 43 42 41 39 53 50	85				1.00E+01	1.55E+06	1.55E+05
Isobutyraldehyde	78-84-2	5 min	3	1.23	9: 43 42 41 57 39 55 51 38 37	78	Pungent, Malt, Green	Spicy		4.07E-02	1.84E+06	4.51E+07
Methyl mercaptan	74-93-1	68 h	3	1.27	2: 47 48	87	Sulfur, Gasoline, Garlic	Decomposing, Cabbage, Garlic			1.86E+04	
Acetaldehyde	75-07-0	68 h	4	1.28	2: 44 43	80	Pungent, Ether	Pungent, Ethereal, Aldehydic, Fruity		1.86E-01	2.67E+04	1.44E+05
Isoprene	78-79-5	1 h	3	1.33	1: 67	71					1.73E+04	
		68 h	5	1.34	TIC	88					1.38E+04	
4-methyldecane	2847-72-5	5 min	4	1.39	9: 43 42 71 41 57 39 56 85 51	67					4.31E+05	
		1 h	5	1.40	10: 39 57 55 41 86 53 69 38 52 67	66					1.35E+06	
2-methylpentane	107-83-5	5 min	5	1.40	2: 57 86	97					4.02E+05	
		1 h	4	1.40	8: 43 71 42 41 57 50 56 86	98					1.54E+06	
		68 h	6	1.40	7: 43 42 41 71 67 70 72	96					2.15E+05	
2,3,4-trimethylpentane	565-75-3	68 h	7	1.41	3: 43 39 71	80					1.77E+05	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

							Published Descriptors		Published ODT (ppm)			
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
Isocyanatomethane	624-83-9	5 min	6	1.44	2: 39 70	68					3.68E+04	
		68 h	9	1.45	3: 57 56 67	78					3.85E+04	
Ethylenimine	151-56-4	5 min	7	1.45	3: 42 43 55	76					1.94E+04	
		1 h	7	1.53	1: 41	70					5.22E+04	
2-methylaziridine	75-55-8	5 min	8	1.45	TIC	83					3.61E+04	
		68 h	8	1.45	1: 56	78					4.85E+04	
3-methylpentane	96-14-0	5 min	9	1.45	3: 56 57 53	91					1.05E+05	
		1 h	6	1.45	5: 57 56 55 58 86	98					4.24E+05	
		68 h	10	1.46	TIC	90					2.24E+04	
Propanal	123-38-6	68 h	11	1.57	TIC	75	Solvent, Pungent	Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty		2.69E-02	2.79E+04	1.04E+06
Butane	106-97-8	68 h	13	1.65	8: 43 58 42 39 53 57 41 44	83				2.04E+02	4.69E+06	2.30E+04
1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide	1447-71-8	68 h	14	1.66	4: 37 59 60 55	73					3.29E+05	
Acetone	67-64-1	5 min	10	1.66	2: 58 43	89		Solvent		1.45E+01	7.49E+04	5.18E+03
		1 h	8	1.65	5: 43 42 39 41 37	96		Solvent		1.45E+01	4.78E+05	3.30E+04
		68 h	12	1.65	TIC	99		Solvent		1.45E+01	5.35E+06	3.70E+05
Methacrolein	78-85-3	68 h	15	2.13	TIC	95		Wild hyacinth foliage			1.40E+05	
Formic acid	64-18-6	68 h	16	2.33	3: 45 72 42	69		Acetic		2.82E+01	6.40E+05	2.27E+04
Ethanol	64-17-5	5 min	11	2.34	2: 45 43	91	Sweet	Alcoholic		2.88E+01	7.27E+04	2.52E+03
		68 h	17	2.34	6: 45 43 46 72 42 41	93	Sweet	Alcoholic		2.88E+01	8.83E+05	3.06E+04
Methylene chloride	75-09-2	5 min	12	2.42	4: 84 51 49 86	93				2.82E+01	4.51E+04	1.60E+03
		1 h	9	2.43	2: 47 49	98				2.82E+01	2.81E+05	9.98E+03
		68 h	18	2.43	3: 84 49 51	94				2.82E+01	7.21E+04	2.56E+03
Pentanal	110-62-3	68 h	19	3.66	TIC	84	Almond, Malt, Pungent	Fermented		6.03E-03	6.40E+04	1.06E+07

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

							Published Descriptors		Published ODT (ppm)			
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
tert-butanol	75-65-0	5 min	13	3.91	1: 59	67		Camphor			2.32E+04	
		68 h	23	3.94	2: 33 41	74		Camphor			5.49E+04	
Ethylenediamine	107-15-3	5 min	14	3.92	TIC	73					1.04E+05	
		68 h	21	3.93	TIC	73					1.13E+05	
1,1-dimethyl-hydrazine	57-14-7	5 min	15	3.93	TIC	79					5.44E+04	
		68 h	20	3.92	TIC	79					3.19E+05	
Hydrazine	302-01-2	5 min	16	3.95	1: 33	76		Ammoniacal		3.00E+00	1.58E+03	5.26E+02
		68 h	22	3.93	1: 33	77				3.00E+00	5.33E+03	1.78E+03
Hexanal	66-25-1	68 h	24	5.99	4: 44 42 67 40	96	Grass, Tallow, Fat	Green		1.38E-02	5.52E+05	4.00E+07
1-butanol	71-36-3	68 h	25	6.12	TIC	93	Medicine, Fruit	Fermented		4.90E-01	5.54E+04	1.13E+05
Nonane	111-84-2	68 h	26	6.70	11: 41 71 85 70 39 129 83 42 98 53 45	95	Alkane	Gasoline		1.26E+00	5.78E+05	4.59E+05
Sabinene	3387-41-5	5 min	17	7.90	4: 93 79 107 106	82	Pepper, Turpentine, Wood	Woody			6.25E+04	
α-phellandrene	99-83-2	5 min	19	7.90	TIC	87	Turpentine, Mint, Spice	Terpenic			5.43E+04	
		1 h	12	7.92	13: 94 91 93 55 51 136 92 79 121 77 108 103 122	90	Turpentine, Mint, Spice	Terpenic			8.87E+04	
		68 h	27	7.93	11: 93 91 55 92 94 79 41 136 77 107 105	86	Turpentine, Mint, Spice	Terpenic			2.28E+05	
α-pinene	80-56-8	5 min	18	7.90	TIC	85	Pine, Turpentine	Herbal		6.92E-01	5.43E+04	7.85E+04
		1 h	13	7.93	8: 93 81 68 107 43 105 95 78	93	Pine, Turpentine	Herbal		6.92E-01	3.65E+05	5.28E+05
		68 h	28	7.93	TIC	92	Pine, Turpentine	Herbal		6.92E-01	1.24E+05	1.80E+05
γ-terpinene	99-85-4	5 min	20	7.90	4: 93 53 136 41	74	Gasoline, Turpentine	Terpenic			9.27E+04	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
2-isopropenyl-3-methylpyrazine	145984-65-2	5 min	21	7.90	1: 134	67					7.52E+03	
(+)-4-Carene	29050-33-7	1 h	10	7.91	5: 105 119 121 80 136	67			4.00E+00		7.28E+04	1.82E+04
Betahistine	5638-76-6	1 h	11	7.91	8: 136 93 80 43 41 106 65 94	70					5.56E+05	
2-heptanone	110-43-0	68 h	29	8.45	TIC	93	Soap	Cheesy		1.41E-01	2.14E+05	1.51E+06
Isoamyl alcohol	123-51-3	68 h	30	8.61	4: 67 53 39 85	67	Whiskey, Malt, Burnt	Fusel oil, Alcoholic, Whiskey, Fruity, Banana		4.47E-02	1.41E+05	3.17E+06
Heptanal	111-71-7	68 h	31	8.62	13: 42 69 71 55 39 81 86 45 96 85 53 54 65	97	Fat, Citrus, Rancid	Green		4.79E-03	1.22E+06	2.54E+08
4-methylpyrimidine	3438-46-8	68 h	32	9.06	4: 94 67 51 42	91					1.75E+05	
4-pyridinamine	504-24-5	68 h	33	9.06	TIC	88					7.41E+04	
1,3,5-triazine-2,4,6-triamine	108-78-1	5 min	22	9.27	1: 126	67					2.43E+03	
Styrene	100-42-5	68 h	34	9.45	4: 103 78 51 83	92	Balsamic, Gasoline	Balsamic		1.45E-01	5.62E+04	3.89E+05
Myrcene	123-35-3	1 h	14	9.93	TIC	92	Balsamic, Must, Spice	Peppery, Terpene, Spicy, Balsam, Plastic	1.30E-02		2.88E+05	2.22E+07
		68 h	35	9.94	17: 94 137 66 82 89 42 115 70 119 54 61 107 122 76 57 56 62	94	Balsamic, Must, Spice	Peppery, Terpene, Spicy, Balsam, Plastic	1.30E-02		6.31E+06	4.85E+08
β-pinene	18172-67-3	68 h	36	9.97	17: 70 121 43 54 38 56 122 62 106 89 83 134 61 137 76 75 120	97	Pine, Resin, Turpentine	Terpenic			1.67E+07	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
Dimethylpyrazine	123-32-0	68 h	37	10.63	TIC	71	Cocoa, Roasted nut, Roast beef, Medicine	Cocoa, Roasted nuts, Roast Beef, Woody, Grass, Medical			7.94E+03	
1-hexanol	111-27-3	68 h	38	10.74	4: 56 69 42 84	85	Resin, Flower, Breen	Herbal		4.37E-02	1.38E+05	3.15E+06
Camphene	79-92-5	1 h	16	10.89	12: 91 53 67 65 121 107 80 105 93 77 41 95	87	Camphor	Woody			4.38E+05	
		68 h	40	10.91	TIC	89	Camphor	Woody			1.38E+06	
Limonene	138-86-3	5 min	23	10.89	3: 93 67 68	68	Lemon, Orange	Citrus		4.37E-01	1.42E+04	3.26E+04
		1 h	15	10.89	12: 91 53 67 65 121 107 80 105 93 77 41 95	92	Lemon, Orange	Citrus		4.37E-01	4.38E+05	1.00E+06
		68 h	39	10.91	TIC	95	Lemon, Orange	Citrus		4.37E-01	1.38E+06	3.17E+06
Piperidine	110-89-4	68 h	41	11.20	2: 44 57	67		Animal		3.72E-01	1.71E+05	4.61E+05
Octanal	124-13-0	68 h	42	11.21	TIC	89	Fat, Soap, Lemon, Green	Aldehydic, Waxy, Citrus, Orange peel, Green, Fatty		1.35E-03	1.43E+05	1.06E+08
m-cymene	535-77-3	68 h	43	11.38	TIC	91					3.47E+04	
Methylisohexenyl ketone	110-93-0	68 h	44	11.54	TIC	95	Pepper, Mushroom, Rubber	Citrus		3.80E-02	1.15E+06	3.04E+07
δ-3-carene	13466-78-9	68 h	45	11.63	TIC	97	Lemon, Resin	Citrus	4.00E+00		1.30E+06	3.25E+05
1-butoxy-2-propanol	5131-66-8	68 h	46	11.77	2: 57 75	67					5.72E+04	
2-butoxyethanol	111-76-2	68 h	47	11.77	TIC	83				3.39E-01	5.08E+04	1.50E+05
Undecane	1120-21-4	68 h	48	11.89	8: 42 84 85 156 113 55 112 39	95	Alkane			1.17E+00	5.89E+05	5.01E+05
Acetic acid	64-19-7	68 h	49	12.23	6: 45 43 60 42 41 61	99	Sour	Acidic		1.45E-01	4.07E+06	2.82E+07

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

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Furfural	98-01-1	68 h	50	12.70	6: 95 96 67 97 38 37	97	Bread, Almond, Sweet	Sweet, Woody, Almond, Baked bread		7.76E-01	1.44E+05	1.86E+05
Citronellolformate	105-85-1	68 h	51	13.09	11: 69 41 105 65 77 54 51 138 96 42 81	70		Floral			2.96E+05	
1,3-dichlorobenzene	541-73-1	68 h	52	13.16	8: 111 50 113 74 149 55 112 75	99					4.74E+05	
2-ethylhexanol	104-76-7	1 h	17	13.81	TIC	87	Rose, Green	Citrus		2.45E-01	1.48E+05	6.05E+05
		68 h	53	13.83	15: 57 41 121 43 71 136 70 83 84 55 98 39 69 81 53	86	Rose, Green	Citrus		2.45E-01	8.30E+05	3.38E+06
5-methylindane	874-35-1	68 h	54	13.90	9: 132 92 115 131 73 91 133 65 128	82					4.21E+05	
2-ethenyl-1,3-dimethylbenzene	2039-90-9	68 h	55	13.91	7: 115 45 102 129 114 82 39	87					2.52E+05	
Benzaldehyde	100-52-7	1 h	18	14.08	TIC	98	Almond, Burnt sugar	Fruity		4.17E-02	8.98E+05	2.15E+07
		68 h	56	14.06	11: 106 105 77 51 52 76 53 39 38 62 36	99	Almond, Burnt sugar	Fruity		4.17E-02	1.90E+07	4.55E+08
2-chloro acetophenone	532-27-4	5 min	24	14.12	2: 77 105	75				2.57E-02	4.00E+03	1.56E+05
		1 h	19	14.08	6: 105 51 77 52 78 63	78				2.57E-02	6.57E+05	2.56E+07
		68 h	57	14.07	6: 57 60 49 43 61 86	77				2.57E-02	4.11E+05	1.60E+07
Dodecane	112-40-3	68 h	58	14.21	20: 57 55 41 59 122 83 112 72 113 93 70 170 98 67 127 95 97 193 171 58	70	Alkane	Alkane		2.04E+00	2.11E+06	1.03E+06
tert-butyl-benzene	98-06-6	68 h	59	14.49	7: 92 117 119 120 115 131 66	89					1.24E+05	

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SI Table 2 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
Linalool	78-70-6	1 h	20	15.12	TIC	91	Flower, Lavender	Floral		5.37E-02	3.31E+05	6.16E+06
		68 h	60	15.14	19: 71 93 43 41 69 80 121 67 82 65 83 72 81 111 107 105 136 39 79	98	Flower, Lavender	Floral		5.37E-02	1.92E+06	3.57E+07
cis-2-pinanol	4948-29-2	1 h	21	15.43	TIC	72		Herbal			1.30E+04	
Benzonitrile	100-47-0	68 h	61	15.46	TIC	87	Rancid, Sweet				7.23E+04	
α-ionol	25312-34-9	68 h	62	15.67	TIC	81		Ionone, Tropical, Sweet, Floral, Violet, Woody			8.15E+05	
Fenchyl alcohol	1632-73-1	1 h	22	15.72	TIC	78	Camphor	Camphor, Borneol, Pine, Woody, Dry, Sweet, Lemon			5.65E+04	
2-ethoxyethanol	110-80-5	68 h	63	15.78	2: 45 60	69				1.23E+00	3.10E+04	2.52E+04
Decanal	112-31-2	68 h	64	15.90	12: 43 82 57 71 83 56 70 95 39 72 128 97	93	Soap, Orange peel, Tallow	Aldehydic		8.91E-04	5.62E+05	6.30E+08
Methyl heptadienone	1604-28-0	68 h	65	15.91	17: 55 41 71 81 43 54 77 42 110 44 56 85 96 79 53 65 128	72		Cinnamon, Coconut, Spice, Woody, Sweet, Weedy			4.69E+05	
Methyl benzoate	93-58-3	68 h	66	16.25	4: 115 51 77 130	75	Prune, Lettuce, Herb, Sweet	Phenolic		1.07E-01	2.73E+04	2.55E+05
Tridecane	629-50-5	68 h	67	16.38	15: 57 43 55 85 141 84 56 99 58 86 69 83 127 39 53	92	Alkane	Alkane		2.14E+00	5.78E+05	2.70E+05
Acetophenone	98-86-2	68 h	68	16.50	5: 77 226 51 163 50	92	Musty, Flower, Almond	Floral		3.63E-01	2.09E+05	5.74E+05
Salicyladehyde	90-02-8	68 h	69	16.82	3: 91 121 93	68		Medicinal		7.41E-03	1.33E+04	1.80E+06
Benzyl formate	104-57-4	68 h	70	17.06	4: 136 90 91 119	71		Floral			3.64E+04	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

							Published Descriptors		Published ODT (ppm)			
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
2-methyl-1H-imidazole	693-98-1	68 h	71	17.13	4: 82 148 43 81	68					2.64E+04	
α-terpineol	98-55-5	1 h	23	17.74	TIC	80	Oil, Anise, Mint	Floral		3.72E-02	3.75E+04	1.01E+06
		68 h	72	17.74	17: 136 59 112 139 81 92 67 95 122 79 68 80 78 121 54 105 51	91	Oil, Anise, Mint	Floral		3.72E-02	4.43E+05	1.19E+07
Acetamide	60-35-5	68 h	73	17.88	1: 43	70		Mousy		6.03E+01	5.33E+04	8.85E+02
Benzyl acetate	140-11-4	68 h	74	18.05	5: 107 91 90 108 150	80	Fresh, Boiled vegetable	Sweet, Floral, Fruity, Jasmine, Fresh		1.45E-01	8.01E+04	5.54E+05
Verbenone	80-57-9	1 h	24	18.16	TIC	75		Camphor, Menthol, Celery			9.46E+03	
DL-carvone	99-49-0	68 h	75	18.71	4: 108 54 93 79	70	Mint, Basil, Fennel	Minty, Licorice		2.24E-02	6.11E+04	2.73E+06
Methyl acetylsalicylate	580-02-9	68 h	76	18.88	6: 121 152 153 64 65 43	93					2.13E+05	
Methyl salicylate	119-36-8	68 h	77	18.88	TIC	93	Peppermint	Minty		4.37E-02	1.31E+05	3.00E+06
(+)-sativene	3650-28-0	1 h	25	19.70	20: 93 69 120 148 106 68 55 92 189 95 149 175 135 162 190 136 83 91 53 103	75					2.37E+07	
Tyramine	51-67-2	1 h	27	19.73	6: 51 85 38 62 90 75	70		Meaty			9.20E+06	
β-caryophyllene	87-44-5	68 h	78	19.74	3: 122 56 110	83	Wood, Spice	Spice	6.40E-02		4.77E+06	7.46E+07
Benzyl Alcohol	100-51-6	5 min	25	19.75	7: 107 79 51 108 89 105 78	89	Sweet, Flower	Floral			2.31E+05	
		1 h	26	19.71	11: 78 53 109 149 39 129 66 65 123 134 202	96	Sweet, Flower	Floral			2.16E+07	
		68 h	79	19.77	TIC	100	Sweet, Flower	Floral			1.47E+08	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
α-terpinene	99-86-5	68 h	80	20.00	15: 105 80 94 136 106 68 91 161 40 65 189 43 55 135 83	70	Lemon	Woody			3.84E+05	
α-longipinene	5989-08-2	68 h	81	20.02	19: 121 136 119 161 122 91 55 81 41 67 135 39 189 78 80 53 137 56 82	76					6.13E+05	
Phenylethyl alcohol	60-12-8	68 h	82	20.38	3: 92 122 91	76	Honey, Spice, Rose, Lilac	Floral		1.70E-02	4.48E+04	2.64E+06
2-methyl naphthalene	91-57-6	68 h	83	20.44	7: 142 116 141 139 221 115 211	93		Floral			2.47E+05	
α-humulene	6753-98-6	1 h	28	20.55	20: 93 80 121 107 79 92 147 91 70 41 105 109 205 94 122 189 106 82 204 95	98	Wood	Wood	1.20E-01		3.99E+06	3.32E+07
		68 h	84	20.57	20: 93 121 80 67 92 189 147 94 204 91 53 41 107 95 106 79 55 161 109 77	97	Wood	Wood	1.20E-01		3.65E+06	3.04E+07
Benzyl nitrile	140-29-4	68 h	85	20.71	2: 90 116	71					8.20E+04	
α-cubebene	17699-14-8	68 h	86	20.92	4: 161 105 119 193	66	Herb, Wax	Herb			3.82E+04	
β-selinene	17066-67-0	1 h	29	21.28	17: 147 205 68 133 161 148 189 105 175 93 107 135 109 123 53 69 134	95	Herb	Herb			6.66E+05	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

							Published Descriptors		Published ODT (ppm)		
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
		68 h	87	21.29	20: 95 160 81 135 108 80 149 67 119 106 41 109 205 175 94 53 141 136 52 190	98	Herb	Herb			2.92E+06	
Aromadendrene	489-39-4	1 h	32	21.70	TIC	71	Wood	Wood			8.73E+04	
		68 h	88	21.30	20: 91 79 108 107 105 121 93 204 161 95 81 119 145 92 147 67 83 106 122 77	79	Wood	Wood			3.56E+06	
α-guaiene	3691-12-1	1 h	30	21.38	TIC	72	Wood, Balsamic	Wood			3.36E+05	
		68 h	92	21.72	20: 121 204 148 107 83 122 120 129 189 84 115 79 41 77 106 95 133 53 147 55	79	Wood, Balsamic	Wood			1.32E+06	
α-gurjunene	489-40-7	1 h	31	21.40	TIC	88	Wood, Balsamic	Wood			2.34E+05	
		68 h	89	21.44	20: 69 41 91 109 134 108 43 92 149 65 147 189 135 206 52 119 96 120 42 136	86	Wood, Balsamic	Wood			7.00E+06	
β-cedrene	546-28-1	68 h	90	21.45	11: 69 148 41 94 67 96 92 80 136 53 68	76					1.93E+06	
Phenol	108-95-2	68 h	91	21.64	TIC	90	Phenolic	Phenolic		1.10E-01	2.37E+05	2.16E+06
Dyclocaine	586-60-7	1 h	33	21.70	8: 120 105 67 109 122 121 91 119	66					1.69E+05	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
		68 h	93	21.74	6: 83 145 123 104 95 159	67					2.71E+05	
(+)-calarene	17334-55-3	1 h	34	21.79	17: 147 109 161 91 148 204 135 133 92 189 107 94 93 159 134 41 149	78					6.42E+05	
		68 h	94	21.81	20: 161 204 147 162 108 133 106 105 91 107 65 176 67 95 160 135 150 189 109 41	84					2.84E+06	
α-cedrene	469-61-4	1 h	35	22.09	15: 119 204 161 93 65 69 133 80 121 135 134 41 189 94 79	72		Woody, Cedar, Sweet, Fresh			4.47E+05	
Valencene	4630-07-3	1 h	36	22.20	20: 161 204 131 133 91 53 106 190 68 108 43 66 77 94 162 78 148 73 160 143	96	Green, Oil	Citrus			3.46E+06	
		68 h	95	22.25	20: 161 133 135 91 93 119 51 107 67 81 77 104 41 55 63 175 108 136 94 132	96	Green, Oil	Citrus			8.12E+06	
γ-gurjunene	22567-17-5	1 h	37	22.30	20: 93 147 77 105 129 108 79 189 119 81 91 135 106 175 131 145 205 51 95 109	92		Musty			4.50E+06	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
		68 h	96	22.34	20: 161 122 204 107 105 91 93 81 149 67 77 108 147 148 109 134 120 106 65 136	92		Musty			4.02E+07	
Dimethylbenzylcarbinyl acetate	151-05-3	68 h	97	22.43	TIC	72		Sweet, Floral, Fruity, Rose, Green, Pear, Berry, Jasmine, Powdery			1.42E+06	
2,6-dimethylquinoline	877-43-0	68 h	98	23.17	15: 157 153 200 218 164 158 156 115 63 68 105 91 128 201 139	74					3.28E+05	
2-phenoxyethanol	122-99-6	68 h	99	23.76	18: 94 138 77 79 39 119 95 91 45 51 232 50 78 92 182 96 75 125	94		Mild, Rose, Balsam, Cinnamyl			1.18E+06	
erolidol	7212-44-4	68 h	100	23.98	20: 69 41 81 43 79 163 108 121 123 136 97 91 178 120 119 94 140 160 133 155	78	Wood, Flower, Wax	Floral			2.92E+06	
(+)-nerolidol	142-50-7	68 h	101	23.99	20: 69 107 123 80 163 110 133 161 91 150 120 162 68 119 105 95 77 70 92 149	80		Floral			3.11E+06	
Caryophyllene oxide	1139-30-6	1 h	38	24.09	TIC	74	Herb, Sweet, Spice	Woody			2.69E+04	
		68 h	102	24.11	TIC	90	Herb, Sweet, Spice	Woody			1.99E+06	
Methyl anthranilate	134-20-3	68 h	103	25.23	5: 120 119 151 98 65	87	Honey, Flower	Fruity		1.15E-03	5.83E+04	5.07E+07

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 2 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
2,4-di-tert-butylphenol	96-76-4	68 h	104	26.37	3: 191 74 206	74		Phenolic			1.37E+05	
α-bisabolol	72691-24-8	1 h	39	26.43	TIC	77					3.95E+04	
		68 h	105	26.45	20: 109 43 41 95 121 94 71 147 122 55 68 148 81 77 91 80 56 97 190 134	98					6.77E+06	
(-)-Globulol	489-41-8	68 h	106	27.33	8: 79 222 190 83 133 92 94 39	73					6.55E+05	
Diethyl Phthalate	84-66-2	68 h	107	27.45	12: 149 177 122 76 176 105 222 121 75 194 178 151	97					1.62E+06	
Benzophenone	119-61-9	68 h	108	28.79	TIC	85		Balsam, Rose, Metallic, Powdery, Geranium			7.99E+04	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 Summary of VOCs emitted from unpackaged marijuana into headspace and captured by SPME during 5 min, 1h, 68 h static sampling at room temperature.

							Published Descriptors		Published ODT (ppm)		
Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Flavornet[23]	TGSC[24]	LRI & Odour Database[25]	Devos, *et al.*[26]	PAC	OAV
Ethylene oxide	75-21-8	68 h	1	1.06	2: 44 46	66				8.51E+02	1.13E+06	1.33E+03
Butyl formate	592-84-7	1 h	1	1.13	3: 41 39 56	65		Fruity			2.32E+04	
		68 h	2	1.13	2: 39 56	67		Fruity			8.34E+03	
Acetaldehyde	75-07-0	1 h	2	1.20	2: 43 42	88	Pungent, Ether	Pungent, Ethereal, Aldehydic, Fruity		1.86E-01	8.62E+03	4.63E+04
Isobutane	75-28-5	5 min	1	1.23	12: 43 42 41 57 72 39 50 55 58 54 56 37	84				1.00E+01	1.21E+06	1.21E+05
		68 h	3	1.24	9: 43 42 41 56 71 53 61 37 58	85				1.00E+01	2.27E+06	2.27E+05
		1 h	3	1.24	10: 43 42 41 57 39 72 55 56 73 37	85				1.00E+01	2.94E+06	2.94E+05
Methyl mercaptan	74-93-1	68 h	4	1.27	3: 47 48 45	84	Sulfur, Gasoline, Garlic	Decomposing, Cabbage, Garlic			1.13E+04	
Isoprene	78-79-5	68 h	5	1.33	3: 67 68 39	86					5.78E+04	
		1 h	4	1.34	TIC	93					3.12E+04	
2-methylpentane	107-83-5	5 min	2	1.39	3: 71 43 42	97					2.82E+05	
		1 h	5	1.40	12: 42 41 55 39 69 72 70 86 56 40 65 50	97					6.18E+05	
		68 h	6	1.40	10: 43 41 71 70 42 57 55 39 86 56	97					3.99E+05	
3,4,5-trimethyl-1-hexene	56728-10-0	5 min	3	1.40	4: 41 86 39 70	68					2.59E+05	
		1 h	6	1.40	TIC	67					6.20E+05	
2,3,4-trimethylpentane	565-75-3	1 h	7	1.40	9: 43 70 41 55 57 53 56 54 50	77					2.03E+05	
3-methylpentane	96-14-0	5 min	4	1.45	2: 56 57	86					7.49E+04	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
		68 h	7	1.45	TIC	93					5.09E+04	
		1 h	8	1.46	TIC	97					1.22E+05	
2-methylaziridine	75-55-8	1 h	9	1.46	5: 57 56 41 53 39	81					1.67E+05	
Dimethylsulfide	75-18-3	1 h	10	1.51	5: 46 45 47 61 35	94	Cabbage, Sulfur, Gasoline	Sulfury, Onion, Sweet corn, Vegetable, Cabbage, Tomato, Green, Radish		2.24E-03	9.43E+04	4.21E+07
		68 h	8	1.51	1: 47	88	Cabbage, Sulfur, Gasoline	Sulfury, Onion, Sweet corn, Vegetable, Cabbage, Tomato, Green, Radish		2.24E-03	4.04E+04	1.80E+07
Propanal	123-38-6	1 h	11	1.57	TIC	76	Solvent, Pungent	Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty		2.69E-02	3.30E+04	1.23E+06
		68 h	9	1.57	1: 58	75	Solvent, Pungent	Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty		2.69E-02	4.70E+04	1.75E+06
Butane	106-97-8	1 h	12	1.65	5: 41 59 44 37 60	84				2.04E+02	1.88E+06	9.21E+03
Acetone	67-64-1	5 min	5	1.65	TIC	83		Solvent		1.45E+01	7.16E+04	4.95E+03
		1 h	13	1.66	10: 43 58 42 39 41 38 37 44 36 59	99		Solvent		1.45E+01	4.98E+06	3.45E+05
		68 h	10	1.65	6: 43 58 42 39 41 44	99		Solvent		1.45E+01	1.97E+06	1.36E+05
Isobutyraldehyde	78-84-2	1 h	14	1.77	TIC	88	Pungent, Malt, Green	Spicy		4.07E-02	1.52E+04	3.73E+05
Methacrolein	78-85-3	1 h	15	2.14	TIC	87		Wild hyacinth foliage			3.42E+04	
		68 h	11	2.13	TIC	96		Wild hyacinth foliage			1.13E+05	
Ethanol	64-17-5	5 min	6	2.33	2: 45 46	95	Sweet	Alcoholic		2.88E+01	1.70E+05	5.90E+03

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

							Published Descriptors		Published ODT (ppm)			
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
		1 h	16	2.33	6: 45 46 39 42 41 47	99	Sweet	Alcoholic		2.88E+01	3.01E+05	1.04E+04
		68 h	12	2.34	2: 45 42	91	Sweet	Alcoholic		2.88E+01	3.02E+05	1.05E+04
Methylene chloride	75-09-2	1 h	17	2.42	5: 84 39 86 88 47	95				2.82E+01	7.08E+04	2.51E+03
Pentanal	110-62-3	68 h	13	3.66	TIC	68	Almond, Malt, Pungent	Fermented		6.03E-03	9.80E+03	1.63E+06
tert-butanol	75-65-0	5 min	8	3.94	TIC	75		Camphor			3.37E+04	
		68 h	14	3.92	5: 33 43 59 40 57	77		Camphor			4.49E+05	
3-pentanol	584-02-1	1 h	19	3.92	TIC	71	Fruit	Herbal		4.68E-01	1.21E+05	2.58E+05
Ethylenediamine	107-15-3	5 min	7	3.93	TIC	76					1.94E+05	
1,1-dimethyl-hydrazine	57-14-7	5 min	9	3.94	TIC	79					9.60E+04	
		1 h	18	3.91	TIC	83					1.41E+05	
		68 h	15	3.93	3: 60 58 45	91					1.01E+05	
Hydrazine	302-01-2	5 min	10	3.96	2: 33 61	77		Ammoniacal		3.00E+00	3.41E+03	1.14E+03
		1 h	20	3.92	3: 33 45 37	77				3.00E+00	4.44E+03	1.48E+03
		68 h	16	3.93	2: 33 61	77				3.00E+00	1.03E+04	3.42E+03
Hexanal	66-25-1	1 h	21	5.99	TIC	84	Grass, Tallow, Fat	Green		1.38E-02	3.44E+04	2.49E+06
		68 h	17	5.98	9: 41 43 56 44 55 57 40 50 54	96	Grass, Tallow, Fat	Green		1.38E-02	7.43E+05	5.39E+07
1-butanol	71-36-3	68 h	18	6.12	TIC	91	Medicine, Fruit	Fermented		4.90E-01	4.11E+04	8.39E+04
Nonane	111-84-2	68 h	19	6.68	TIC	87	Alkane	Gasoline		1.26E+00	4.14E+04	3.29E+04
2-isopropenyl-3-methylpyrazine	145984-65-2	1 h	22	7.67	4: 135 75 134 133	73					1.03E+05	
α-phellandrene	99-83-2	5 min	12	7.89	TIC	82	Turpentine, Mint, Spice	Terpenic			2.36E+04	
		1 h	25	7.90	11: 92 136 91 93 108 78 39 77 107 106 66	79	Turpentine, Mint, Spice	Terpenic			1.55E+06	
(+)-4-Carene	29050-33-7	1 h	23	7.90	13: 121 78 136 68 103 117 80 52 51 77 106 107 81	82			4.00E+00		2.20E+05	5.49E+04
Sabinene	3387-41-5	1 h	26	7.92	7: 91 67 107 108 41 94 63	69	Pepper, Turpentine, Wood	Woody			1.09E+05	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

							Published Descriptors			Published ODT (ppm)		
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
γ-terpinene	99-85-4	1 h	27	7.92	7: 77 107 80 121 92 137 63	69	Gasoline, Turpentine	Terpenic			1.64E+05	
α-pinene	80-56-8	5 min	11	7.89	TIC	79	Pine, Turpentine	Herbal		6.92E-01	2.36E+04	3.41E+04
		1 h	24	7.90	11: 92 136 91 93 108 78 39 77 107 106 66	97	Pine, Turpentine	Herbal		6.92E-01	4.88E+05	7.05E+05
		68 h	20	7.92	7: 80 91 121 92 79 105 107	93	Pine, Turpentine	Herbal		6.92E-01	1.88E+05	2.71E+05
2-heptanone	110-43-0	68 h	21	8.44	TIC	90	Soap	Cheesy		1.41E-01	2.35E+05	1.66E+06
Heptanal	111-71-7	68 h	22	8.61	TIC	97	Fat, Citrus, Rancid	Green		4.79E-03	1.90E+06	3.97E+08
4-methylpyrimidine	3438-46-8	68 h	23	9.05	TIC	90					7.71E+04	
4-pyridinamine	504-24-5	68 h	24	9.05	4: 67 52 53 41	86					1.03E+05	
1,3,5-triazine-2,4,6-triamine	108-78-1	5 min	13	9.26	2: 126 84	68					4.66E+03	
Styrene	100-42-5	68 h	25	9.42	3: 104 102 50	92	Balsamic, Gasoline	Balsamic		1.45E-01	1.32E+05	9.11E+05
Myrcene	123-35-3	1 h	28	9.92	TIC	94	Balsamic, Must, Spice	Peppery, Terpene, Spicy, Balsam, Plastic	1.30E-02		6.11E+05	4.70E+07
		68 h	26	9.93	9: 137 50 117 103 74 89 51 58 138	96	Balsamic, Must, Spice	Peppery, Terpene, Spicy, Balsam, Plastic	1.30E-02		9.74E+06	7.49E+08
β-pinene	18172-67-3	68 h	27	9.94	TIC	97	Pine, Resin, Turpentine	Terpenic			1.62E+07	
Dimethylpyrazine	123-32-0	68 h	28	10.61	TIC	70	Cocoa, Roasted nut, Roast beef, Medicine	Cocoa, Roasted nuts, Roast Beef, Woody, Grass, Medical			6.43E+03	
1-hexanol	111-27-3	68 h	29	10.73	4: 42 56 41 84	80	Resin, Flower, Breen	Herbal		4.37E-02	2.08E+05	4.75E+06
Diacetone alcohol	123-42-2	1 h	29	10.80	2: 59 43	77				8.91E-01	5.51E+04	6.18E+04
		68 h	30	10.80	1: 101	71				8.91E-01	8.98E+04	1.01E+05

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

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Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
Camphene	79-92-5	1 h	30	10.89	7: 79 68 136 107 92 95 91	84	Camphor	Woody			1.33E+05	
		68 h	32	10.89	TIC	89	Camphor	Woody			1.23E+06	
Limonene	138-86-3	1 h	31	10.90	6: 68 92 80 136 69 41	90	Lemon, Orange	Citrus		4.37E-01	1.71E+05	3.92E+05
		68 h	31	10.89	TIC	95	Lemon, Orange	Citrus		4.37E-01	1.23E+06	2.83E+06
Octanal	124-13-0	68 h	33	11.20	TIC	85	Fat, Soap, Lemon, Green	Aldehydic, Waxy, Citrus, Orange peel, Green, Fatty		1.35E-03	1.07E+05	7.96E+07
m-cymene	535-77-3	1 h	32	11.36	TIC	86					3.49E+04	
		68 h	34	11.37	TIC	92					1.22E+05	
Methylisohexenyl ketone	110-93-0	1 h	33	11.54	TIC	80	Pepper, Mushroom, Rubber	Citrus		3.80E-02	4.51E+04	1.19E+06
		68 h	35	11.52	13: 93 58 67 111 56 71 42 53 38 82 54 44 70	97	Pepper, Mushroom, Rubber	Citrus		3.80E-02	1.48E+06	3.90E+07
δ-3-carene	13466-78-9	68 h	36	11.62	TIC	97	Lemon, Resin	Citrus	4.00E+00		1.49E+06	3.72E+05
2-butoxyethanol	111-76-2	68 h	37	11.75	7: 45 87 41 42 75 39 88	89				3.39E-01	1.41E+05	4.16E+05
Undecane	1120-21-4	68 h	38	11.87	TIC	92	Alkane			1.17E+00	1.31E+05	1.12E+05
Acetic acid	64-19-7	1 h	34	12.25	3: 43 44 207	100	Sour	Acidic		1.45E-01	7.66E+05	5.30E+06
		68 h	39	12.21	7: 43 45 60 44 40 207 59	99	Sour	Acidic		1.45E-01	6.49E+06	4.49E+07
Furfural	98-01-1	68 h	40	12.68	2: 96 39	96	Bread, Almond, Sweet	Sweet, Woody, Almond, Baked bread		7.76E-01	1.64E+05	2.11E+05
Citronellolformate	105-85-1	68 h	41	13.08	7: 120 41 92 96 93 109 138	71		Floral			4.20E+05	
1,3-dichlorobenzene	541-73-1	68 h	42	13.15	6: 75 111 84 76 150 147	97					3.07E+05	
2-ethylhexanol	104-76-7	1 h	35	13.80	7: 84 41 54 112 43 56 70	91	Rose, Green	Citrus		2.45E-01	3.39E+05	1.38E+06

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

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Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
		68 h	43	13.83	TIC	92	Rose, Green	Citrus		2.45E-01	1.28E+06	5.22E+06
2-ethenyl-1,3-dimethylbenzene	2039-90-9	68 h	44	13.93	4: 104 89 117 115	81					6.28E+04	
Benzaldehyde	100-52-7	5 min	15	14.11	2: 106 77	87	Almond, Burnt sugar	Fruity		4.17E-02	4.75E+04	1.14E+06
		1 h	36	14.06	TIC	98	Almond, Burnt sugar	Fruity		4.17E-02	1.00E+06	2.40E+07
		68 h	45	14.05	14: 106 105 51 78 107 52 74 39 75 79 63 37 108 36	99	Almond, Burnt sugar	Fruity		4.17E-02	3.24E+07	7.76E+08
2-chloroacetophenone	532-27-4	5 min	14	14.09	2: 105 52	68				2.57E-02	2.00E+04	7.80E+05
Dodecane	112-40-3	68 h	46	14.19	8: 170 98 84 85 127 147 58 269	68	Alkane	Alkane		2.04E+00	4.12E+05	2.02E+05
1-(3-methylphenyl)-ethanone	585-74-0	68 h	47	14.46	TIC	85					3.97E+04	
tert-butyl-benzene	98-06-6	68 h	48	14.48	8: 79 117 119 78 134 135 92 120	87					1.37E+05	
Linalool	78-70-6	1 h	37	15.12	20: 93 69 80 71 72 122 41 92 55 107 136 65 94 53 81 105 45 56 96 82	95	Flower, Lavender	Floral		5.37E-02	3.68E+05	6.85E+06
		68 h	50	15.13	20: 41 43 69 121 80 106 67 83 92 39 94 79 72 97 68 136 57 96 82 107	98	Flower, Lavender	Floral		5.37E-02	3.65E+06	6.79E+07
Isobornyl thiocyanoacetate	115-31-1	68 h	49	15.12	15: 39 96 109 154 42 56 84 95 65 85 139 58 54 44 57	73					2.51E+06	
cis-2-pinanol	4948-29-2	1 h	38	15.41	TIC	79		Herbal			1.66E+04	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

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Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
Benzonitrile	100-47-0	68 h	51	15.47	2: 103 91	80	Rancid, Sweet				1.56E+05	
α-ionol	25312-34-9	68 h	52	15.66	19: 138 95 67 79 43 39 86 77 123 42 96 91 139 41 93 71 55 137 44	80		Ionone, Tropical, Sweet, Floral, Violet, Woody			1.08E+06	
Fenchyl alcohol	1632-73-1	1 h	39	15.73	TIC	72	Camphor	Camphor, Borneol, Pine, Woody, Dry, Sweet, Lemon			1.94E+04	
2-ethoxyethanol	110-80-5	68 h	53	15.79	3: 104 59 72	67				1.23E+00	1.06E+05	8.63E+04
Decanal	112-31-2	68 h	54	15.89	TIC	84	Soap, Orange peel, Tallow	Aldehydic		8.91E-04	1.45E+05	1.63E+08
Methyl heptadienone	1604-28-0	68 h	55	15.91	TIC	86		Cinnamon, Coconut, Spice, Woody, Sweet, Weedy			7.94E+04	
Methyl benzoate	93-58-3	68 h	56	16.25	1: 105	82	Prune, Lettuce, Herb, Sweet	Phenolic		1.07E-01	3.90E+04	3.64E+05
Tridecane	629-50-5	68 h	57	16.35	4: 70 84 73 56	82	Alkane	Alkane		2.14E+00	1.38E+05	6.47E+04
Acetophenone	98-86-2	68 h	58	16.51	3: 105 90 106	87	Musty, Flower, Almond	Floral		3.63E-01	7.91E+04	2.18E+05
Salicyladehyde	90-02-8	68 h	59	16.81	TIC	67		Medicinal		7.41E-03	2.70E+04	3.64E+06
Benzyl formate	104-57-4	68 h	60	17.04	6: 91 136 90 89 78 51	92		Floral			1.69E+05	
2-methyl-1H-imidazole	693-98-1	68 h	61	17.12	3: 82 97 54	82					3.89E+04	
α-terpineol	98-55-5	1 h	40	17.73	TIC	80	Oil, Anise, Mint	Floral		3.72E-02	2.54E+04	6.84E+05
		68 h	62	17.73	8: 121 68 81 136 107 77 109 69	93	Oil, Anise, Mint	Floral		3.72E-02	9.94E+05	2.68E+07
Acetamide	60-35-5	68 h	63	17.89	10: 146 69 128 117 120 45 115 105 161 134	87		Mousy		6.03E+01	3.78E+05	6.28E+03
Benzyl acetate	140-11-4	68 h	64	18.03	9: 150 109 108 91 79 107 51 50 83	94	Fresh, Boiled vegetable	Sweet, Floral, Fruity, Jasmine, Fresh		1.45E-01	2.68E+05	1.85E+06

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SI Table 3 continued

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m-tert-butylphenol	585-34-2	1 h	41	18.15	5: 135 80 108 79 91	68					6.76E+04	
		68 h	65	18.15	8: 108 107 79 91 150 115 39 110	69					2.05E+04	
p-tert-butylphenol	98-54-4	1 h	42	18.15	TIC	68		Leathery			1.54E+04	
Verbenone	80-57-9	1 h	43	18.16	TIC	82		Camphor, Menthol, Celery			2.55E+04	
		68 h	66	18.16	8: 107 91 149 55 146 150 73 108	68		Camphor, Menthol, Celery			5.53E+04	
DL-carvone	99-49-0	68 h	67	18.68	4: 107 82 54 93	82	Mint, Basil, Fennel	Minty, Licorice		2.24E-02	1.56E+05	6.97E+06
Methyl acetylsalicylate	580-02-9	68 h	68	18.86	4: 82 125 120 43	90					5.82E+04	
Methyl salicylate	119-36-8	68 h	69	18.87	5: 120 152 121 43 63	88	Peppermint	Minty		4.37E-02	1.09E+05	2.50E+06
β-caryophyllene	87-44-5	5 min	16	19.67	TIC	92	Wood, Spice	Spice	6.40E-02		3.14E+05	4.91E+06
		1 h	44	19.65	10: 134 124 96 66 112 190 122 110 177 138	89	Wood, Spice	Spice	6.40E-02		1.05E+06	1.64E+07
		68 h	70	19.69	20: 133 93 69 120 41 147 148 67 189 81 94 95 175 82 135 162 137 129 122 136	80	Wood, Spice	Spice	6.40E-02		5.25E+06	8.20E+07
(+)-sativene	3650-28-0	68 h	71	19.72	3: 105 86 37	73					1.40E+07	
Tyramine	51-67-2	5 min	18	19.74	3: 80 51 49	70		Meaty			6.64E+05	
		1 h	46	19.73	5: 90 62 109 37 61	70		Meaty			3.71E+06	
Benzyl Alcohol	100-51-6	5 min	17	19.73	5: 90 80 91 51 74	97	Sweet, Flower	Floral			5.67E+05	
		1 h	45	19.72	TIC	96	Sweet, Flower	Floral			5.83E+06	
		68 h	72	19.79	11: 79 107 51 91 63 109 74 49 40 48 155	100	Sweet, Flower	Floral			1.86E+08	

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Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
α-terpinene	99-86-5	68 h	73	19.98	15: 121 109 122 136 161 162 123 41 120 107 81 91 190 204 92	67	Lemon	Woody			2.09E+05	
α-longipinene	5989-08-2	68 h	74	20.01	4: 119 109 91 40	73					4.73E+05	
Dimethylsulfone	67-71-0	1 h	47	20.11	2: 94 79	80	Sulfur, Burnt	Sulfurous, Burnt			1.93E+04	
		68 h	75	20.10	7: 94 81 82 54 119 46 150	82	Sulfur, Burnt	Sulfurous, Burnt			1.54E+05	
Phenylethyl alcohol	60-12-8	68 h	76	20.39	5: 91 122 92 44 57	82	Honey, Spice, Rose, Lilac	Floral		1.70E-02	4.72E+04	2.78E+06
2-methyl naphthalene	91-57-6	68 h	77	20.43	5: 141 139 115 205 147	81		Floral			6.87E+04	
α-humulene	6753-98-6	5 min	19	20.53	TIC	83	Wood	Wood	1.20E-01		4.30E+04	3.58E+05
		1 h	48	20.52	19: 92 79 94 105 95 91 148 63 65 204 120 41 123 82 135 78 66 39 128	97	Wood	Wood	1.20E-01		1.42E+06	1.19E+07
		68 h	78	20.56	20: 136 106 94 119 204 55 190 82 115 95 161 54 189 149 148 52 71 128 65 66	97	Wood	Wood	1.20E-01		5.44E+06	4.53E+07
Benzyl nitrile	140-29-4	68 h	79	20.70	5: 51 117 112 118 77	88					1.13E+05	
α-cubebene	17699-14-8	68 h	80	20.90	TIC	71	Herb, Wax	Herb			2.41E+04	
β-selinene	17066-67-0	1 h	50	21.25	15: 161 162 134 94 190 43 91 81 204 121 123 95 92 131 175	72	Herb	Herb			1.56E+05	
		68 h	82	21.26	20: 55 79 91 147 96 120 176 121 135 105 106 175 145 190 81 94 104 40 109 148	98	Herb	Herb			3.65E+06	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
α-gurjunene	489-40-7	1 h	51	21.38	10: 147 131 107 133 109 204 119 79 95 105	81	Wood, Balsamic	Wood			1.34E+05	
		68 h	81	21.11	13: 204 93 161 127 189 133 95 122 169 128 190 117 123	89	Wood, Balsamic	Wood			4.08E+05	
β-cedrene	546-28-1	68 h	83	21.41	20: 161 93 134 107 77 122 94 41 121 120 67 106 95 66 54 39 135 163 108 119	76					1.62E+06	
Phenol	108-95-2	68 h	84	21.63	17: 94 66 65 47 62 95 63 64 40 38 74 90 55 61 49 53 36	93	Phenolic	Phenolic		1.10E-01	2.08E+06	1.89E+07
Aromadendrene	489-39-4	1 h	49	21.25	TIC	91	Wood	Wood			1.16E+05	
		68 h	85	21.70	19: 121 204 189 83 120 105 148 122 147 91 79 93 107 119 95 134 157 54 103	77	Wood	Wood			1.81E+06	
α-guaiene	3691-12-1	68 h	86	21.71	20: 133 120 91 106 105 119 78 148 204 189 93 83 161 107 123 145 67 80 81 53	78	Wood, Balsamic	Wood			7.32E+05	
α-cedrene	469-61-4	1 h	52	22.07	TIC	72		Woody, Cedar, Sweet, Fresh			1.74E+04	
		68 h	87	22.10	20: 93 119 79 204 107 94 95 77 136 69 81 189 120 39 205 122 106 161 148 133	74		Woody, Cedar, Sweet, Fresh			6.98E+06	
Valencene	4630-07-3	5 min	20	22.18	TIC	76	Green, Oil	Citrus			1.85E+04	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

Compound	CAS	Ext. Time	Peak #	RT (min)	Models	Net % Match	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, *et al.*[26]	PAC	OAV
		1 h	53	22.19	TIC	95	Green, Oil	Citrus			8.47E+05	
		68 h	88	22.21	19: 133 67 205 77 55 162 190 189 175 130 109 174 92 121 117 106 94 108 80	95	Green, Oil	Citrus			1.39E+07	
γ-gurjunene	22567-17-5	1 h	54	22.27	TIC	89		Musty			5.08E+05	
		68 h	89	22.32	20: 122 105 91 121 81 41 149 55 123 190 65 175 129 104 103 73 51 173 163 150	92		Musty			4.82E+07	
Dimethylbenzylcarbinyl acetate	151-05-3	68 h	90	22.41	6: 71 132 117 60 59 115	65		Sweet, Floral, Fruity, Rose, Green, Pear, Berry, Jasmine, Powdery			8.36E+05	
2,6-dimethylquinoline	877-43-0	68 h	91	23.13	15: 157 142 127 136 156 200 155 135 158 115 152 128 129 153 126	70					5.20E+05	
2-phenoxyethanol	122-99-6	68 h	92	23.77	6: 94 77 66 147 65 71	90		Mild, Rose, Balsam, Cinnamyl			1.63E+05	
Nerolidol	7212-44-4	68 h	93	23.96	20: 41 119 81 136 71 95 121 67 79 105 123 91 135 80 108 163 190 109 53 124	83	Wood, Flower, Wax	Floral			3.53E+06	
(+)-nerolidol	142-50-7	68 h	94	23.97	20: 69 93 107 81 202 55 79 121 109 161 123 67 133 53 178 77 137 163 204 97	86		Floral			3.42E+06	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 3 continued

							Published Descriptors			Published ODT (ppm)	
Compound	**CAS**	**Ext. Time**	**Peak #**	**RT (min)**	**Models**	**Net % Match**	**Flavornet[23]**	**TGSC[24]**	**LRI & Odour Database[25]**	**Devos, *et al.*[26]**	**PAC**	**OAV**
Caryophyllene oxide	1139-30-6	68 h	95	24.09	20: 95 82 83 69 123 66 124 105 159 71 161 189 138 111 160 191 97 112 162 54	91	Herb, Sweet, Spice	Woody			3.19E+06	
Methyl anthranilate	134-20-3	68 h	96	25.24	8: 93 80 92 151 65 120 98 95	86	Honey, Flower	Fruity		1.15E-03	8.93E+04	7.78E+07
2,4-di-tert-butylphenol	96-76-4	68 h	97	26.36	4: 191 200 116 206	74		Phenolic			7.61E+04	
α-bisabolol	72691-24-8	68 h	98	26.42	20: 204 95 110 67 122 92 139 84 81 148 161 97 137 133 68 123 78 83 140 190	98					7.43E+06	
(-)-Globulol	489-41-8	68 h	99	27.32	18: 81 121 151 119 95 123 204 133 91 148 222 189 145 55 149 41 79 82	73					8.23E+05	
Diethyl Phthalate	84-66-2	68 h	100	27.43	7: 149 65 222 50 119 150 93	93					4.00E+05	
Benzophenone	119-61-9	68 h	101	28.78	2: 105 93	80		Balsam, Rose, Metallic, Powdery, Geranium			9.39E+04	

A total of 121 chemical peaks were tentatively identified by *multidimensional* GC-MS; associated published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. Peak # refers to chronological order compounds eluted from the analytical GC column; RT refers to retention time in min; Quantifying Ions are the component ions (number of ions used to quantify: corresponding m/z in order of relative abundance) or total ion chromatogram (TIC) used in AMDIS target library search and signal integration; % Match is net percent probability match of unknown spectra to database spectra, calculated by AMDIS; PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value (Eq. 1), assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes.

SI Table 4. Summary of F-statistics and p-values from two-way analysis of variance comparing the effect of packaging on VOC emitted from marijuana at 5 min, 1 h, and 68 h extraction times.

				Packaging		Ext. Time	
Compound	R^2	F-Statistic	p-value	F-Statistic	p-value	F-Statistic	p-value
(-)-Globulol	0.987	51.765	0.019	1	0.423	77.148	0.013†
(+)-4-Carene	0.817	2.98	0.261	1	0.423	3.97	0.201
(+)-calarene	0.657	1.275	0.468	1.824	0.309	1	0.5
(+)-nerolidol	0.998	310.437	0.003	1	0.423	465.156	0.002†
(+)-sativene	0.302	0.288	0.834	0.085	0.798	0.39	0.719
1-(3-methylphenyl)-ethanone	0.6	1	0.535	1	0.423	1	0.5
1,1-dimethyl-hydrazine	0.423	0.489	0.725	0.012	0.922	0.728	0.579
1,3,5-triazine-2,4,6-triamine	0.914	7.097	0.126	1	0.423	10.145	0.09
1,3-dichlorobenzene	0.957	14.855	0.064	1	0.423	21.782	0.044◊
1-butanol	0.979	30.556	0.032	1	0.423	45.335	0.022†
1-butoxy-2-propanol	0.6	1	0.535	1	0.423	1	0.5
1-hexanol	0.961	16.559	0.057	1	0.423	24.338	0.039†
1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide	0.6	1	0.535	1	0.423	1	0.5
2,3,4-trimethylpentane	0.254	0.227	0.872	0.006	0.943	0.338	0.748
2,4-di-tert-butylphenol	0.927	8.506	0.107	1	0.423	12.259	0.075
2,6-dimethylquinoline	0.952	13.284	0.071	1	0.423	19.425	0.049◊
2-butoxyethanol	0.834	3.353	0.238	1	0.423	4.529	0.181
2-chloroacetophenone	0.712	1.646	0.4	3.183	0.216	0.878	0.533
2-ethenyl-1,3-dimethylbenzene	0.766	2.18	0.33	1	0.423	2.771	0.265
2-ethoxyethanol	0.793	2.554	0.294	1	0.423	3.331	0.231
2-ethylhexanol	0.962	16.695	0.057	2.675	0.244	23.706	0.040‡
2-heptanone	0.998	295.779	0.003	1	0.423	443.169	0.002†
2-isopropenyl-3-methylpyrazine	0.558	0.842	0.583	0.796	0.466	0.864	0.536
2-methyl naphthalene	0.785	2.428	0.305	1	0.423	3.142	0.241
2-methyl-1H-imidazole	0.965	18.596	0.051	1	0.423	27.395	0.035†
2-methylaziridine	0.303	0.289	0.833	0.155	0.732	0.357	0.737
2-methylpentane	0.73	1.803	0.376	0.753	0.477	2.328	0.3
2-nitropropane	0.715	1.676	0.395	3.028	0.224	1	0.5
2-phenoxyethanol	0.692	1.497	0.424	1	0.423	1.746	0.364
3,4,5-trimethyl-1-hexene	0.699	1.552	0.415	2.655	0.245	1	0.5
3-methylpentane	0.712	1.652	0.399	0.985	0.426	1.986	0.335
3-pentanol	0.6	1	0.535	1	0.423	1	0.5
4-methyldecane	0.678	1.406	0.441	2.219	0.275	1	0.5
4-methylpyrimidine	0.877	4.774	0.178	1	0.423	6.66	0.131
4-pyridinamine	0.974	25.105	0.039	1	0.423	37.157	0.026†
5-methylindane	0.6	1	0.535	1	0.423	1	0.5
Acetaldehyde	0.415	0.472	0.733	0.322	0.628	0.548	0.646
Acetamide	0.694	1.509	0.422	1	0.423	1.764	0.362

(†, 19 total) indicates significant difference in concentration of VOC at 68 h sampling time from the other two time points Tukey HSD. (‡, 5 total) indicates significant difference in concentration of the VOC between 5 min and 68 h only, (◊, 5 total) indicates no significance between extraction times after the pairwise comparison test. Statistical analysis software: XLStat V 2014.5.01 (New York, NY, USA). Details on statistical tests are on page 57.

SI Table 4 continued

				Packaging		Ext. Time	
Compound	R^2	F-Statistic	p-value	F-Statistic	p-value	F-Statistic	p-value
Acetic acid	0.96	15.92	0.06	2.216	0.275	22.773	0.042‡
Acetone	0.474	0.6	0.674	0.027	0.885	0.887	0.53
Acetophenone	0.845	3.629	0.224	1	0.423	4.943	0.168
Aromadendrene	0.904	6.245	0.141	0.953	0.432	8.891	0.101
Benzaldehyde	0.937	9.852	0.094	1.034	0.416	14.261	0.066
Benzonitrile	0.889	5.319	0.162	1	0.423	7.479	0.118
Benzophenone	0.994	103.841	0.01	1	0.423	155.261	0.006†
Benzyl acetate	0.797	2.624	0.288	1	0.423	3.436	0.225
Benzyl Alcohol	0.977	28.582	0.034	0.235	0.676	42.755	0.023†
Benzyl formate	0.744	1.937	0.358	1	0.423	2.406	0.294
Benzyl nitrile	0.976	26.564	0.036	1	0.423	39.345	0.025†
Betahistine	0.6	1	0.535	1	0.423	1	0.5
Butane	0.376	0.401	0.77	0.23	0.679	0.487	0.673
Butyl formate	0.687	1.466	0.43	2.399	0.262	1	0.5
Camphene	0.988	55.008	0.018	2.939	0.229	81.043	0.012†
Caryophyllene oxide	0.949	12.413	0.075	0.934	0.436	18.152	0.052
cis-2-pinanol	0.986	45.961	0.021	1	0.423	68.441	0.014†
Citronellolformate	0.971	22.408	0.043	1	0.423	33.111	0.029†
Decanal	0.772	2.256	0.322	1	0.423	2.885	0.257
Diacetone alcohol	0.73	1.804	0.376	3.413	0.206	1	0.5
Diethyl Phthalate	0.764	2.161	0.332	1	0.423	2.742	0.267
Dimethylbenzylcarbinyl acetate	0.939	10.246	0.09	1	0.423	14.869	0.063
Dimethylpyrazine	0.989	60.462	0.016	1	0.423	90.193	0.011†
Dimethylsulfide	0.702	1.567	0.412	2.7	0.242	1	0.5
Dimethylsulfone	0.631	1.14	0.499	1.421	0.356	1	0.5
DL-carvone	0.851	3.814	0.215	1	0.423	5.221	0.161
Dodecane	0.73	1.804	0.376	1	0.423	2.206	0.312
Dyclocaine	0.731	1.813	0.375	3.439	0.205	1	0.5
Ethanol	0.571	0.889	0.568	0.052	0.841	1.308	0.433
Ethylene oxide	0.737	1.872	0.367	1.183	0.39	2.217	0.311
Ethylenediamine	0.685	1.449	0.433	0.017	0.909	2.165	0.316
Ethylenimine	0.69	1.484	0.427	2.451	0.258	1	0.5
Fenchyl alcohol	0.824	3.122	0.252	1	0.423	4.183	0.193
Formic acid	0.6	1	0.535	1	0.423	1	0.5
Furfural	0.996	163.606	0.006	1	0.423	244.909	0.004†
Heptanal	0.955	14.188	0.067	1	0.423	20.782	0.046◊
Hexanal	0.981	35.257	0.028	1.63	0.33	52.07	0.019†
Hydrazine	0.956	14.586	0.065	15.147	0.06	14.306	0.065
Isoamyl alcohol	0.6	1	0.535	1	0.423	1	0.5
Isobornyl thiocyanoacetate	0.6	1	0.535	1	0.423	1	0.5
Isobutane	0.706	1.604	0.406	0.194	0.702	2.309	0.302
Isobutyraldehyde	0.595	0.981	0.541	0.975	0.427	0.984	0.504
Isocyanatomethane	0.75	1.998	0.351	3.994	0.184	1	0.5

(†, 19 total) indicates significant difference in concentration of VOC at 68 h sampling time from the other two time points Tukey HSD. (‡, 5 total) indicates significant difference in concentration of the VOC between 5 min and 68 h only, (◊, 5 total) indicates no significance between extraction times after the pairwise comparison test. Statistical analysis software: XLStat V 2014.5.01 (New York, NY, USA). Details on statistical tests are on page 57.

SI Table 4 continued

				Packaging		Ext. Time	
Compound	R^2	F-Statistic	p-value	F-Statistic	p-value	F-Statistic	p-value
Isoprene	0.789	2.499	0.299	2.204	0.276	2.647	0.274
Limonene	0.992	78.567	0.013	3.839	0.189	115.931	0.009†
Linalool	0.909	6.654	0.133	1.066	0.41	9.448	0.096
m-cymene	0.828	3.2	0.247	2.58	0.249	3.51	0.222
Methacrolein	0.954	13.7	0.069	0.024	0.892	20.537	0.046‡
Methyl acetylsalicylate	0.781	2.382	0.309	1	0.423	3.072	0.246
Methyl anthranilate	0.958	15.381	0.062	1	0.423	22.572	0.042◊
Methyl benzoate	0.97	21.864	0.044	1	0.423	32.296	0.030†
Methyl heptadienone	0.713	1.653	0.398	1	0.423	1.98	0.336
Methyl mercaptan	0.946	11.73	0.08	1	0.423	17.095	0.055
Methyl salicylate	0.992	81.765	0.012	1	0.423	122.148	0.008†
Methylene chloride	0.856	3.959	0.208	4.542	0.167	3.668	0.214
Methylisohexenyl ketone	0.986	48.075	0.02	1.466	0.35	71.38	0.014†
m-tert-butylphenol	0.675	1.384	0.445	2.153	0.28	1	0.5
Myrcene	0.959	15.512	0.061	1.308	0.371	22.614	0.042‡
Nerolidol	0.991	74.032	0.013	1	0.423	110.548	0.009†
Nonane	0.647	1.222	0.48	1	0.423	1.332	0.429
Octanal	0.981	33.568	0.029	1	0.423	49.852	0.020†
Pentanal	0.702	1.57	0.412	1	0.423	1.854	0.35
Phenol	0.676	1.389	0.445	1	0.423	1.583	0.387
Phenylethyl alcohol	0.999	993.769	0.001	1	0.423	1490.154	0.001†
Piperidine	0.6	1	0.535	1	0.423	1	0.5
Propanal	0.871	4.514	0.187	3.29	0.211	5.126	0.163
p-tert-butylphenol	0.6	1	0.535	1	0.423	1	0.5
Sabinene	0.309	0.297	0.829	0.097	0.785	0.398	0.715
Salicyladehyde	0.902	6.126	0.144	1	0.423	8.689	0.103
Styrene	0.87	4.465	0.188	1	0.423	6.197	0.139
tert-butanol	0.672	1.367	0.449	1.082	0.408	1.51	0.398
tert-butyl-benzene	0.998	280.293	0.004	1	0.423	419.939	0.002†
Tridecane	0.759	2.102	0.338	1	0.423	2.653	0.274
Tyramine	0.833	3.319	0.24	0.68	0.496	4.638	0.177
Undecane	0.748	1.984	0.352	1	0.423	2.476	0.288
Valencene	0.883	5.022	0.171	0.181	0.712	7.442	0.118
Verbenone	0.668	1.341	0.454	2.092	0.285	0.966	0.509
α-bisabolol	0.998	288.108	0.003	0.832	0.458	431.746	0.002†
α-cedrene	0.564	0.862	0.576	0.827	0.459	0.88	0.532
α-cubebene	0.952	13.256	0.071	1	0.423	19.384	0.049◊
α-guaiene	0.939	10.314	0.09	3.26	0.213	13.841	0.067
α-gurjunene	0.636	1.163	0.493	1.047	0.414	1.222	0.45
α-humulene	0.813	2.896	0.267	0.037	0.865	4.326	0.188
α-ionol	0.981	33.639	0.029	1	0.423	49.958	0.020†
α-longipinene	0.984	40.155	0.024	1	0.423	59.733	0.016†
α-phellandrene	0.535	0.767	0.609	0.564	0.531	0.869	0.535

(†, 19 total) indicates significant difference in concentration of VOC at 68 h sampling time from the other two time points Tukey HSD. (‡, 5 total) indicates significant difference in concentration of the VOC between 5 min and 68 h only, (◊, 5 total) indicates no significance between extraction times after the pairwise comparison test. Statistical analysis software: XLStat V 2014.5.01 (New York, NY, USA). Details on statistical tests are on page 57.

SI Table 4 continued

				Packaging		Ext. Time	
Compound	R^2	F-Statistic	p-value	F-Statistic	p-value	F-Statistic	p-value
α-pinene	0.965	18.134	0.053	1.343	0.366	26.529	0.036‡
α-terpinene	0.923	7.96	0.114	1	0.423	11.44	0.08
α-terpineol	0.872	4.56	0.185	0.935	0.435	6.372	0. 136
β-caryophyllene	0.995	133.751	0.007	7.561	0.111	196.847	0.005†
β-cedrene	0.992	84.259	0.012	1	0.423	125.888	0.008†
β-pinene	1	2781.634	0	1	0.423	4171.951	0.000†
β-selinene	0.971	22.028	0.044	0.041	0.858	33.021	0.029†
γ-gurjunene	0.985	44.322	0.022	0.143	0.742	66.412	0.015†
γ-terpinene	0.31	0.3	0.827	0.1	0.782	0.4	0.714
δ-3-carene	0.995	144.384	0.007	1	0.423	216.076	0.005†

(†, 19 total) indicates significant difference in concentration of VOC at 68 h sampling time from the other two time points Tukey HSD. (‡, 5 total) indicates significant difference in concentration of the VOC between 5 min and 68 h only, (◊, 5 total) indicates no significance between extraction times after the pairwise comparison test. Statistical analysis software: XLStat V 2014.5.01 (New York, NY, USA). Details on statistical tests are on page 57.

A two-way analysis of variance (ANOVA) was performed without replication and assuming no interaction, followed by a multiple comparisons test. Normal distribution and equal variance is assumed for the analysis. The two-way ANOVA without repetition was conducted to compare the effect of packaging on VOCs emitted from marijuana at 5 min, 1hr, and 68hr extraction times using static headspace SPME extraction at room temperature. Just one single measurement was taken at each combination of factors; therefore it is assumed that there were no interactions between the independent variables of sampling time and packaging. The post hoc Tukey honest significant difference (HSD) is conservative and attempts to control the overall alpha level, and is less sensitive than the ANOVA, so this could account for the 5 VOC showing no significant difference in the pairwise comparison, but indicated as significant in the ANOVA.

A Wilcoxon signed rank test of paired samples was performed (SI Table 5). The hypothesized difference between volatile compound abundance and odor activity value was assumed to be zero, with a 5% significance level. Test interpretation: H_0: The two samples follow the same distribution. H_a: The distributions of the two samples are different. If the computed p-value is lower than the significance level alpha=0.05, one should reject the null hypothesis H_0, and accept the alternative hypothesis H_a. . Statistical analysis software: XLStat V 2014.5.01 (New York, NY, USA).

SI Table 5. Wilcoxon signed rank test of paired samples.

Plastic Bag (5 min)	
V	30
Expected value	27.500
Variance (V)	96.250
p-value (Two-tailed)	0.838
alpha	0.05

Loose (5 min)	
V	15
Expected value	22.500
Variance (V)	71.250
p-value (Two-tailed)	0.407
alpha	0.05

Plastic Bag (1 h)	
V	22
Expected value	52.500
Variance (V)	253.750
p-value (Two-tailed)	0.060
alpha	0.05

Loose (1 h)	
V	71
Expected value	162.500
Variance (V)	1381.250
p-value (Two-tailed)	0.014
alpha	0.05

Plastic Bag (68 h)	
V	245
Expected value	663.000
Variance (V)	11381.500
p-value (Two-tailed)	**< 0.0001**
alpha	0.05

Loose (68 h)	
V	143
Expected value	540.500
Variance (V)	8377.750
p-value (Two-tailed)	**< 0.0001**
alpha	0.05

SI Table 6. Hierarchy of volatile compounds with published ODT, emitted from marijuana, through packaging over 68 at room temperature.

	Plastic Bag 5 min		Plastic Bag 1 h		Plastic Bag 68 h		Loose 5 min		Loose 1 h		Loose 68 h		Duffel Bag 68 h	
Compound	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV
Hydrazine	1	1			1	3	1	1	1	1	2	2	3	1
Salicyladehyde					2	28					3	28	23	39
Acetaldehyde					3	10			2	5				
Methyl benzoate					4	15					4	17	40	32
Propanal					5	26			5	16	8	23		
2-ethoxyethanol					6	7					13	8		
Phenylethyl alcohol					7	30					9	26	27	35
2-butoxyethanol					8	11					19	19		
Acetamide					9	1					28	3		
1-butanol					10	9					6	7	4	5
Styrene					11	19					17	20		
Methyl anthranilate					12	45					11	40	13	47
DL-carvone					13	31					21	31		
Pentanal					14	37					1	21		
Methylene chloride	5	2	5	2	15	4			9	2				
Benzyl acetate					16	23					26	24		
α-pinene	6	8	8	5	17	13	3	4	17	14	23	16	49	25
Methyl salicylate					18	32					15	25	14	23
1-hexanol					19	33					24	29	12	22
Isoamyl alcohol					20	35								
Octanal					21	47					14	41		
Furfural					22	14					22	13		
Piperidine					23	21							28	17
Acetophenone					24	24					10	14	17	14
2-heptanone					25	27					25	22	19	18
Phenol					26	29					39	33	24	21
2-chloroacetophenone	2	9	11	13	27	39	2	7					51	52
α-terpineol			2	9	28	38			4	13	31	34	48	42
Hexanal					29	44			6	18	30	38	5	20
Decanal					30	51					20	43	39	55
Tridecane					31	16					18	6	7	3
Nonane					32	20					7	5		
Undecane					33	22					16	10		
Formic acid					34	5							36	4
2-ethylhexanol			4	6	35	36			15	17	34	30		
Ethanol	7	5			36	8	7	3	14	4	27	4	42	6
Methylisohexenyl ketone					37	41			7	15	35	35		
Ethylene oxide	9	3			38	2					32	1		

Numbers in the table are the assigned ranking of the compound in terms of concentration ([Conc]) or odor impact (OAV) as calculated by Eq. 1. A rank of 1 indicates low concentration (e.g., Hydrazine from 5 min, plastic bag) or low odor impact (e.g., 2-nitropropane from 1 h, plastic bag). A rank of 56 indicates high concentration (e.g., Limonene from 68 h, duffel bag) or high odor impact (e.g., Nonanal from 68 h, duffel bag).

SI Table 6 continued

Compound	Plastic Bag 5 min		Plastic Bag 1 h		Plastic Bag 68 h		Loose 5 min		Loose 1 h		Loose 68 h		Duffel Bag 68 h	
	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV
Heptanal					39	48					37	44		
δ-3-carene					40	17					36	18		
Limonene	4	7	9	8	41	34			12	12	33	27	56	45
Isobutane			14	7	42	12	9	5	24	9	40	15	54	16
Linalool			7	10	43	43			16	20	41	39	37	37
Dodecane					44	25					29	12	43	15
α-humulene			13	14	45	42	4	6	22	21	43	37		
Acetic acid					46	40			19	19	44	36	53	41
Butane					47	6			23	3			46	2
β-caryophyllene					48	46	8	9	21	22	42	42		
Acetone	8	6	10	4	49	18	6	2	25	10	38	11	47	9
Myrcene			6	12	50	50			18	25	45	45		
Benzaldehyde			12	11	51	49	5	8	20	23	46	46	52	46
Dimethylsulfide									10	24	5	32		
Diacetone alcohol									8	7	12	9		
Piperonal													1	19
Acrolein													2	7
Nerol													6	51
Thymol													8	27
Carvacrol													9	29
p-xylene													10	10
o-guaiacol													11	49
o-methylacetophenone													15	38
Eugenol													16	34
Cumene													18	28
p-cymene													20	44
1,2,3,4-tetramethylbenzene													21	30
p-methylacetophenone													22	40
o-xylene													25	12
Durene													26	31
Methyl heptanoate													29	26
o-cymene													30	54
Anethole													31	43
Nitrobenzene													32	33
Toluene													33	13
Ethylacetate													34	11
2-butanone													35	8
Linalyl acetate													38	48
1-undecanol													41	36
3-pentanol									11	8			44	24
Propylamine													45	50
Nonanal													50	56

Numbers in the table are the assigned ranking of the compound in terms of concentration ([Conc]) or odor impact (OAV) as calculated by Eq. 1. A rank of 1 indicates low concentration (e.g., Hydrazine from 5 min, plastic bag) or low odor impact (e.g., 2-nitropropane from 1 h, plastic bag). A rank of 56 indicates high concentration (e.g., Limonene from 68 h, duffel bag) or high odor impact (e.g., Nonanal from 68 h, duffel bag).

SI Table 6 continued

Compound	Plastic Bag 5 min		Plastic Bag 1 h		Plastic Bag 68 h		Loose 5 min		Loose 1 h		Loose 68 h		Duffel Bag 68 h	
	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV	[Conc]	OAV
Isobutyraldehyde	10	10							3	11			55	53
2-nitropropane	3	4	1	1										
(+)-4-Carene			3	3					13	6				

Numbers in the table are the assigned ranking of the compound in terms of concentration ([Conc]) or odor impact (OAV) as calculated by Eq. 1. A rank of 1 indicates low concentration (e.g., Hydrazine from 5 min, plastic bag) or low odor impact (e.g., 2-nitropropane from 1 h, plastic bag). A rank of 56 indicates high concentration (e.g., Limonene from 68 h, duffel bag) or high odor impact (e.g., Nonanal from 68 h, duffel bag).

SI Table 7. Correlation coefficients between concentration and odor impact of volatile compounds emitted from marijuana.

		R^2 (Plastic bag)			R^2 (Loose)			R^2 (Duffel bag)
X variable	Y variable	5 min	1 h	68 h	5 min	1 h	68 h	68 h
Rank of [Conc]	Rank of OAV	0.235	0.4211	0.1118	0.2284	0.1976	0.1693	0.1047
Rank of [Conc]	[OAV]	0.2717	0.4123	0.1444	0.1001	0.172	0.1772	0.1001
[Conc]	Rank of OAV	0.1062	0.3804	0.1397	0.223	0.1182	0.2232	0.1043
[Conc]	[OAV]	0.5888	0.2061	0.2806	0.1333	0.1183	0.638	0.0981

Scatter plots were generated for all combinations of rank of OAV and rank of concentration (SI Table 6), actual concentration (peak area counts of mass detector, assuming equal response for all compounds) and calculated OAV (Eq. 1), and correlation coefficients of the best fit line are given in SI Table 7. Correlation coefficients between concentration and odor impact of volatile compounds emitted from marijuana.. The highest correlation was between concentration and calculated OAV (R^2 = 0.638) of volatiles emitted from loose, dry marijuana over 68 h at room temperature; the lowest correlation was between was between concentration and calculated OAV (R^2 = 0.0981) of volatiles emitted from fresh marijuana through a duffel bag over 68 h at room temperature.

SI Table 8. Identification of VOCs emitted though cloth duffel bag in headspace of marijuana sample, and captured by SPME over 68 hours.

SI Table 8 continued

Compound #	Aromagram #	ABC Case	TIC RT (min)		Aromagram RT (min)	Compound	CAS	Published ODT (ppm) LRI & Odour Database[25]	Devos, et al.[26]	Published Descriptors Odor Descriptor	Flavornet[23]	TGSC[24]	PAC	OAV
1		B	1.14			Butyl formate	592-84-7					Fruity	4.89E+04	
2		B	1.24			Isobutane	75-28-5		1.00E+01				6.00E+06	6.00E+05
3		B	1.24	#		Isobutyraldehyde	78-84-2		4.07E-02		Pungent, Malt, Green	Spicy	6.00E+06	1.47E+08
4		B	1.40			2-methylpentane	107-83-5						3.95E+05	
5		B	1.40			4-methyldecane	2847-72-5						3.21E+05	
6		B	1.40			3,4,5-trimethyl-1-hexene	56728-10-0						3.21E+05	
7		B	1.45			2,2,5-trimethylhexane	3522-94-9						5.69E+04	
8		B	1.45			Isocyanatomethane	624-83-9						4.54E+04	
9		B	1.46			3-methylpentane	96-14-0						3.95E+04	
10		B	1.46			2-methylaziridine	75-55-8						8.10E+04	
11		B	1.66	#		Butane	106-97-8		2.04E+02				1.28E+06	6.28E+03
12		B	1.66	#		Acetone	67-64-1		1.45E+01			Solvent	1.28E+06	8.87E+04
13		B	1.77	#		Methyl acetate	79-20-9					Ethereal	2.50E+05	
	1	C			1.92					Plastic, Solvent				
14		B	2.33			Propylene glycol	57-55-6						7.44E+05	
15		B	2.33	#		Ethylacetate	141-78-6		2.63E+00		Pineapple	Ethereal, Fruity, Sweet, Weedy, Green	5.55E+05	2.11E+05
16		B	2.34	#		Ethanol	64-17-5		2.88E+01		Sweet	Alcoholic	1.08E+06	3.74E+04
17		B	2.34			methylhydrazine	60-34-4						7.32E+05	
18		B	2.34	#		Formic acid	64-18-6		2.82E+01			Acetic	7.13E+05	2.53E+04
	2	C			3.09					Onion, Garlic				
	3	C			3.31					Moldy				

Compound # refers to the chronological order of compounds eluted off the analytical GC column; aroma peaks refer to aromagram peak numbers, both from Figure 2. Odor descriptor refers to the descriptors used by panelists in this study. Published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value ((Eq. 1) assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes. # indicates compounds confirmed by pure standard.

SI Table 8 continued

Compound #	Aromagram #	ABC Case	TIC RT (min)		Aromagram RT (min)	Compound	CAS	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, et al.[26]	Published Descriptors: Odor Descriptor	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	PAC	OAV
19		B	3.42			3-methyl-2-cyclopenten-1-one	2758-18-1					Fruity	5.29E+04	
20		B	3.92			Hydrazine	302-01-2		3.00E+00				1.60E+04	5.34E+03
21		B	3.93			Propylamine	107-10-8		1.10E-02			Ammoniacal	1.18E+06	1.08E+08
22		B	3.93			3-pentanol	584-02-1		4.68E-01		Fruit	Herbal	1.18E+06	2.53E+06
23		B	3.93	#		1,1-dimethyl-hydrazine	57-14-7						4.11E+05	
24	4	A	3.93		3.96	Ethylenediamine	107-15-3			Sweet, Solvent			3.89E+05	
25		B	5.05	#		Toluene	108-88-3		1.55E+00		Paint	Sweet	4.51E+05	2.91E+05
26		B	5.06	#		Phenylethyl alcohol	60-12-8		1.70E-02		Honey, Spice, Rose, Lilac	Floral	2.24E+05	1.32E+07
	5	C			5.32					Cardboard				
	6	C			5.50					Sweet, Fruity				
27	7	A	5.99	#	6.00	Hexanal	66-25-1	4.00E-03	1.38E-02	Grassy, Aldehydic	Grass, Tallow, Fat	Green	2.18E+04	1.58E+06
	8	C			6.46					Sweet, Fruity				
	9	C			6.59					Onion, Skunky				
	10	C			6.92					Resiny, **Characteristic**, Onion, Skunky				
	11	C			7.74					Smoky, Resiny, Potato				
	12	C			8.36					Resiny, Potato, **Characteristic**				
28		B	8.42			2-methyl-2-propanamine	75-64-9					0	1.64E+05	
29		B	8.42			Hordenine	539-15-1					0	1.50E+05	
30		B	8.42	#		2-heptanone	110-43-0	1.40E-01	1.41E-01		Soap	Cheesy	1.29E+05	9.14E+05
31		B	8.98			Hexanoic acid, methyl ester	106-70-7				Fruit, Fresh, Sweet	Fruity	3.10E+05	

Compound # refers to the chronological order of compounds eluted off the analytical GC column; aroma peaks refer to aromagram peak numbers, both from Figure 2. Odor descriptor refers to the descriptors used by panelists in this study. Published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value ((Eq. 1) assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes. # indicates compounds confirmed by pure standard.

SI Table 8 continued

Compound #	Aromagram #	ABC Case	TIC RT (min)	Aromagram RT (min)	Compound	CAS	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, et al.[26]	Published Descriptors: Odor Descriptor	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	PAC	OAV
32		B	9.27		Sabinene	3387-41-5				Pepper, Turpentine, Wood	Woody	3.89E+04	
	13	C		9.36					Medicinal, Herbaceous				
	14	C		9.64					Herbaceous, Medicinal				
33	15	B	10.02	9.93	β-pinene	18172-67-3			Aldehydic, Citrus, Mint, **Characteristic**	Pine, Resin, Turpentine	Terpenic	1.65E+08	
34	16	A	10.46	10.48	Isoprene	78-79-5			Moldy			2.38E+05	
35		B	10.53		Furfurylmethylamphetamine	13445-60-8						6.46E+05	
	17	C		10.64					Onion, Garlic, Skunky, Medicinal				
36		B	10.73 #		1-butanol	71-36-3		4.90E-01		Medicine, Fruit	Fermented	1.82E+04	3.71E+04
37		B	10.73 #		1-hexanol	111-27-3		4.37E-02		Resin, Flower, Green	Herbal	9.81E+04	2.25E+06
38		B	10.75 #		Acrolein	107-02-8		1.74E-01			Almond, Cherry	8.29E+03	4.77E+04
39		B	10.90 #		Limonene	138-86-3	1.00E-02	4.37E-01		Lemon, Orange	Citrus	3.48E+07	7.97E+07
40	18	A	10.90 #	10.98	Camphene	79-92-5			Mushroom, Moldy	Camphor	Woody	3.48E+07	
41		B	11.28		(1R)-(+)-trans-isolimonene	5113-87-1						9.34E+05	
42		B	11.37		m-cymene	535-77-3						1.31E+05	
43		B	11.37 #		p-cymene	99-87-6		2.14E-03		Solvent, Gasoline, Citrus	Terpenic	1.31E+05	6.12E+07

Compound # refers to the chronological order of compounds eluted off the analytical GC column; aroma peaks refer to aromagram peak numbers, both from Figure 2. Odor descriptor refers to the descriptors used by panelists in this study. Published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value ((Eq. 1) assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes. # indicates compounds confirmed by pure standard.

SI Table 8 continued

Compound #	Aromagram #	ABC Case	TIC RT (min)	Aromagram RT (min)	Compound	CAS	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, et al.[26]	Published Descriptors: Odor Descriptor	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	PAC	OAV
44		B	11.41		5-ethenyl-2-methylpyridine	140-76-1						3.21E+04	
45		B	11.48		Methyl valerate	624-24-8					Fruity	2.95E+05	
46		B	11.48		Methyl heptanoate	106-73-0		6.92E-02			Fruity	2.48E+05	3.59E+06
47		B	11.52		1,2,3,4-tetramethylbenzene	488-23-3		2.63E-02				1.41E+05	5.36E+06
48	19	A	11.54	11.55	α-phellandrene	99-83-2			Cardboard, Cabbage	Turpentine, Mint, Spice	Terpenic	8.89E+04	
49		B	11.56 #		δ-3-carene	13466-78-9	4.00E+00			Lemon, Resin	Citrus	2.07E+06	
50		B	11.57		α-pinene	80-56-8		6.92E-01		Pine, Turpentine	Herbal	2.20E+06	3.17E+06
	20	C		11.91					Onion, Garlic, Skunky, Sulfury				
51	21	A	12.23 #	12.23	Acetic acid	64-19-7		1.45E-01	Acidic, Burnt, Fatty acid	Sour	Acidic	4.18E+06	2.89E+07
52		B	12.51		(+)-4-Carene	29050-33-7	4.00E+00					5.94E+05	
53		B	12.51		γ-terpinene	99-85-4				Gasoline, Turpentine	Terpenic	5.68E+05	
54		B	12.82 #		2-butanone	78-93-3		7.76E+00		Ether	Ethereal, Fruity, Camphor	6.62E+05	8.52E+04
55		B	13.04		4-methylphenethylamine	3261-62-9						2.00E+05	
56	22	A	13.04	13.04	o-methylacetophenone	577-16-2		6.61E-03	Moldy, Burnt		Floral	1.16E+05	1.76E+07
57		B	13.05		p-methylacetophenone	122-00-9		6.61E-03		Bitter, Almond	Floral	1.69E+05	2.56E+07
58		B	13.06 #		o-xylene	95-47-6		8.51E-01		Geranium	Geranium	1.98E+05	2.33E+05

Compound # refers to the chronological order of compounds eluted off the analytical GC column; aroma peaks refer to aromagram peak numbers, both from Figure 2. Odor descriptor refers to the descriptors used by panelists in this study. Published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value ((Eq. 1) assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes. # indicates compounds confirmed by pure standard.

SI Table 8 continued

Compound #	Aromagram #	ABC Case	TIC RT (min)	Aromagram RT (min)	Compound	CAS	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, et al.[26]	Published Descriptors: Odor Descriptor	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	PAC	OAV
59		B	13.06 #		p-xylene	106-42-3		4.90E-01				6.32E+04	1.29E+05
	23	C		13.37					Moldy, Burnt, Burnt food				
60	24	A	13.59 #	13.63	Nonanal	124-19-6	1.00E-03	2.24E-03	Potato, Resiny, Roasted	Fat, Citrus, Green	Aldehydic	2.37E+06	1.06E+09
61		B	13.81		3,4,5-trimethylphenol	527-54-8					Phenolic	7.55E+05	
62	25	A	13.82	13.86	2-hydroxyacetophenone	118-93-4			Roasted, Potato, Resiny, Moldy		Phenolic	7.57E+04	
63		B	13.87		Isoquinoline	119-65-3					Balsamic	2.30E+04	
64		B	13.89		2-ethenyl-1,3-dimethylbenzene	2039-90-9						1.22E+06	
65		B	13.89		5-methylindane	874-35-1						1.22E+06	
66		B	14.04 #		Benzaldehyde	100-52-7	3.00E-03	4.17E-02		Almond, Burnt sugar	Fruity	3.50E+06	8.40E+07
67		B	14.05		2-chloroacetophenone	532-27-4		2.57E-02				3.08E+06	1.20E+08
	26	C		14.15					Burnt, Burnt food				
68		B	14.17 #		Dodecane	112-40-3		2.04E+00		Alkane	Alkane	1.14E+06	5.58E+05
69		B	14.19 #		α-terpinene	99-86-5				Lemon	Woody	1.43E+06	
70		B	14.19		3-(1-methylethyl)-phenol methylcarbamate	64-00-6						5.04E+05	
71		B	14.21		2,4,6-trimethylphenol	527-60-6					Phenolic	1.08E+06	
72		B	14.21 #		Terpinolene	586-62-9	2.00E-01			Pine, Plastic	Herbal	6.14E+05	
73		B	14.22		tert-butyl-benzene	98-06-6						2.17E+05	
74		B	14.23		o-cymene	527-84-4		7.94E-04				2.54E+05	3.20E+08
75		B	14.23 #		Durene	95-93-2		2.63E-02		Rancid, Sweet	Rancid	1.99E+05	7.58E+06

Compound # refers to the chronological order of compounds eluted off the analytical GC column; aroma peaks refer to aromagram peak numbers, both from Figure 2. Odor descriptor refers to the descriptors used by panelists in this study. Published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value ((Eq. 1) assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes. # indicates compounds confirmed by pure standard.

SI Table 8 continued

Compound #	Aromagram #	ABC Case	TIC RT (min)	Aromagram RT (min)	Compound	CAS	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, et al.[26]	Published Descriptors: Odor Descriptor	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	PAC	OAV
76		B	14.23		Isodurene	527-53-7						1.85E+05	
77		B	14.44		1,2-diethylbenzene	135-01-3						6.97E+05	
78		B	14.45		1,4-diethylbenzene	105-05-5						7.80E+05	
79		B	14.46		3-ethyl-o-xylene	933-98-2						6.77E+05	
	27	C		14.78					Mushroom, Moldy				
80		B	15.11		Linalyl acetate	115-95-7		8.91E-03		Sweet, Fruit	Herbal	8.58E+05	9.62E+07
81		B	15.12		Linalool	78-70-6	6.00E-03	5.37E-02		Flower, Lavender	Floral	8.34E+05	1.55E+07
	28	C		15.28					Moldy, Burnt, Burnt food, Fatty acid				
82		B	15.39		Nerolidol	7212-44-4				Wood, Flower, Wax	Floral	4.33E+04	
83		B	15.40		Limonene dioxide	96-08-2					Mentholic	4.22E+04	
84		B	15.41		Methacrylic anhydride	760-93-0						2.27E+04	
85		B	15.41		Nerol	106-25-2		2.04E-04		Sweet	Floral	2.41E+04	1.18E+08
86		B	15.63 #		o-dimethyl hydroquinone	91-16-7					Vanilla	2.28E+05	
87	29	A	15.64	15.68	4-methyl guaiacol	93-51-6			Herbaceous, Spicy, Burnt food, Fatty Acid, Burnt		Spicy	8.92E+04	
88		B	15.85		1-undecanol	112-42-5		6.76E-02		Mandarin	Waxy	9.21E+05	1.36E+07
89		B	15.85		Decanal	112-31-2	2.00E-03	8.91E-04		Soap, Orange peel, Tallow	Aldehydic	8.90E+05	9.99E+08
90		B	15.86 #		1-hexadecanol	36653-82-4				Flower, Wax	Wax	8.06E+05	
91	30	A	15.90 #	15.90	o-guaiacol	90-05-1		1.00E-03	Medicinal, Herbaceous	Smoke, Sweet, Medicine	Phenolic	9.69E+04	9.69E+07

Compound # refers to the chronological order of compounds eluted off the analytical GC column; aroma peaks refer to aromagram peak numbers, both from Figure 2. Odor descriptor refers to the descriptors used by panelists in this study. Published aroma descriptors from Flavornet[23] and The Good Scents Company (TGSC) [24] and odor detection thresholds (ODT) from LRI & Odour Database[25] and Devos, *et al*.[26] are given. PAC refers peak area counts (i.e. the integrated area under the curve of each chromatographic peak); OAV is the calculated Odor Activity Value ((Eq. 1) assuming equal mass detector response to all compounds, and assuming PAC units of ppm for illustrative purposes. # indicates compounds confirmed by pure standard.

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Compound #	Aromagram #	ABC Case	TIC RT (min)	Aromagram RT (min)	Compound	CAS	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, et al.[26]	Published Descriptors: Odor Descriptor	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	PAC	OAV
92	31	A	16.20	16.18	5-octanolide	698-76-0			Soapy, Citrus, Mint	Peach	Coconut	6.27E+04	
93		B	16.23		Methyl benzoate	93-58-3		1.07E-01		Prune, Lettuce, Herb, Sweet	Phenolic	8.95E+05	8.35E+06
94		B	16.32 #		Tridecane	629-50-5		2.14E+00		Alkane	Alkane	4.28E+04	2.00E+04
95		B	16.35		Propanoic acid, anhydride	123-62-6						8.37E+03	
96		B	16.48		3-ethyltoluene	620-14-4						8.56E+04	
97		B	16.48		p-ethyl toluene	622-96-8						8.56E+04	
98		B	16.48		2-ethyltoluene	611-14-3						7.88E+04	
99		B	16.50		Cumene	98-82-8		2.40E-02				1.18E+05	4.93E+06
100		B	16.50 #		Acetophenone	98-86-2	6.50E-02	3.63E-01		Musty, Flower, Almond	Floral	1.18E+05	3.25E+05
101	32	A	16.50	16.50	Isobutyrophenone	611-70-1			Herbaceous, Medicinal		Green	8.91E+04	
102		B	16.63		Anethole	104-46-1		7.08E-03			Licorice	3.24E+05	4.58E+07
103		B	16.63		Estragole	140-67-0				Licorice, Anise	Anise	3.24E+05	
104		B	16.64		Cuminaldehyde	122-03-2				Acid, Sharp	Spicy	3.97E+05	
105		B	16.64		Pentamethylbenzene	700-12-9						3.97E+05	
106		B	16.65		Benzphentamine	156-08-1						2.82E+05	
107		B	16.65		3-isopropylbenzaldehyde	34246-57-6						3.50E+05	
108		B	16.80		Salicyladehyde	90-02-8		7.41E-03			Medicinal	1.72E+05	2.32E+07
109		B	17.10		Betazole	105-20-4						9.35E+04	
110		B	17.10		2-methyl-1H-imidazole	693-98-1						9.35E+04	
	33	C		17.16					Skunky, Sewer				

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Compound #	Aromagram #	ABC Case	TIC RT (min)	Aromagram RT (min)	Compound	CAS	Published ODT (ppm): LRI & Odour Database[25]	Published ODT (ppm): Devos, et al.[26]	Published Descriptors: Odor Descriptor	Published Descriptors: Flavornet[23]	Published Descriptors: TGSC[24]	PAC	OAV
111		B	17.19		γ-hexalactone	695-06-7				Coumarin, Sweet	Tonka	2.53E+05	
112	34	A	17.41 #	17.40	Piperidine	110-89-4		3.72E-01	Moldy, Burnt food		Animal	2.28E+05	6.13E+05
113		B	17.41		3-methylheptane	589-81-1						1.22E+05	
114		B	17.72		Isobornyl acetate	125-12-2					Balsamic	1.22E+06	
115		B	17.73 #		α-terpineol	98-55-5		3.72E-02		Oil, Anise, Mint	Floral	1.47E+06	3.95E+07
116		B	17.73		Isobornyl thiocyanoacetate	115-31-1						1.03E+06	
117		B	17.76		Hexadecane	544-76-3				Alkane		1.30E+05	
118		B	17.76 #		Pentadecane	629-62-9				Alkane	Waxy	1.30E+05	
	35	C		17.82					Citrus, Herbaceous				
119		B	17.84		Nitrobenzene	98-95-3		4.37E-02				3.81E+05	8.73E+06
	36	C		18.01					Moldy, Burnt food, Burnt				
120		B	18.04		p-acetanisole	100-06-1					Anisic	5.79E+04	
121		B	18.04		3-methyl-5-(1-methylethyl)-Phenol methylcarbamate	2631-37-0						5.79E+04	
122		B	18.04 #		Carvacrol	499-75-2		1.12E-02			Spicy	5.79E+04	5.16E+06
123		B	18.04		Thymol	89-83-8		1.55E-02			Herbal	5.79E+04	3.74E+06
124		B	18.05		m-tert-butylphenol	585-34-2						7.57E+04	
125		B	18.13		α-methylcinnamaldehyde	101-39-3					Spicy	3.89E+05	
	37	C		18.37					Herbaceous, Medicinal				
126		B	18.47		α-cubebene	17699-14-8				Herb, Wax	Herb	3.21E+05	
127		B	18.73		p-aminotoluene	106-49-0						1.57E+03	

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128		B	18.80		1-(3-methylphenyl)-ethanone	585-74-0						1.25E+05	
129		B	18.87 #		Methyl salicylate	119-36-8	4.00E-02	4.37E-02		Peppermint	Minty	1.08E+05	2.48E+06
130		B	19.01		Hexanoic acid, propyl ester	626-77-7				Fruity	Fruity	2.41E+05	
131		B	19.09		(+)-sativene	3650-28-0						8.09E+05	
132		B	19.35		α-longipinene	5989-08-2						5.69E+05	
133		B	19.50		Perillaldehyde	2111-75-3				Spice	Herbal	2.10E+05	
134		B	19.51		(-)-Aristolene	6831-16-9						2.61E+05	
135		B	19.69		β-caryophyllene	87-44-5	6.40E-02			Wood, Spice	Spice	3.85E+07	
	38	C		19.83					Burnt food, Burnt, Piggy, Urinous				
136		B	19.85		α-guaiene	3691-12-1				Wood, Balsamic	Wood	1.68E+06	
137		B	19.96		α-bulnescene	3691-11-0						1.74E+06	
	39	C		20.20					Herbaceous, Smoky				
138	40	A	20.29 #	20.29	β-cedrene	546-28-1			Herbaceous, Citrus			2.34E+06	
139		B	20.30		(+)-nerolidol	142-50-7					Floral	4.48E+06	
140		B	20.43		2-methyl naphthalene	91-57-6					Floral	6.13E+04	
141		B	20.54		α-humulene	6753-98-6	1.20E-01			Wood	Wood	1.23E+07	
142		B	20.68		Benzyl nitrile	140-29-4						2.36E+05	
	41	C		20.73					Herbaceous, Citrus, Resiny				
143		B	20.89		α-copaene	3856-25-5				Wood, Spice	Wood	4.93E+05	
	42	C		21.12					Moldy				
144	43	A	21.26	21.24	β-selinene	17066-67-0			Sweet, Fruity	Herb	Herb	6.06E+06	

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145		B	21.27		(+)-calarene	17334-55-3						1.53E+06	
146		B	21.41		Aromadendrene	489-39-4				Wood	Wood	5.15E+06	
147		B	21.64 #		Phenol	108-95-2		1.10E-01		Phenolic	Phenolic	1.95E+05	1.78E+06
148		B	21.69		Dyclocaine	586-60-7						2.91E+06	
149		B	21.70		Cedryl acetate	77-54-3					Wood	4.85E+05	
150		B	21.77		δ-cadinene	483-76-1				Thyme, Medicine, Wood	Herbal	7.00E+06	
151		B	21.77		α-gurjunene	489-40-7				Wood, Balsamic	Wood	5.25E+06	
	44	C		21.91					Herbaceous, Resiny				
152		B	22.08		Longifolene	475-20-7					Wood	1.43E+06	
	45	C		22.13					Gasoline, Solvent				
153		B	22.22		Valencene	4630-07-3				Green, Oil	Citrus	2.28E+07	
154		B	22.77		γ-gurjunene	22567-17-5					Musty	3.25E+06	
155		B	22.77		α-cadinene	24406-05-1					Wood	6.61E+06	
156	46	A	22.78	22.79	Alloaromadendrene	25246-27-9			Herbaceous, Resiny, Medicinal, **Characteristic**, Piggy, Urinous	Wood	Wood	4.05E+06	
157		B	23.14		2,6-dimethylquinoline	877-43-0						9.79E+05	
158		B	23.23		Tetrahydrozoline	84-22-0						7.06E+05	
159		B	23.98		Propofol	2078-54-8					Phenolic	1.80E+07	
160		B	23.98		Methyl isoeugenol	93-16-3				Clove, Spice	Spice	1.80E+07	
161		B	24.34		Isoeugenol	97-54-1				Flower	Spicy	3.41E+05	
162		B	24.34		Eugenyl acetate	93-28-7					Spicy	2.06E+05	
163		B	24.35		Carbofuran	1563-66-2						1.16E+05	

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164		B	24.35		Eugenol	97-53-0		1.07E-02		Clove, Honey	Spicy	1.16E+05	1.08E+07
165		B	24.51		3-(3-hydroxyphenyl)-2-propenoic acid, methyl ester	3943-95-1						5.39E+04	
	47	C		24.64					Medicinal, Herbaceous, Resiny				
166		B	24.72		Citronellyl acetate	150-84-5				Rose, Dust	Floral	2.78E+05	
	48	C		25.07					Piggy, Urinous, Barnyard				
167		B	25.23		Methyl anthranilate	134-20-3		1.15E-03		Honey, Flower	Fruity	1.04E+05	9.04E+07
168		B	26.36		β-irone	79-70-9					Floral	2.15E+05	
169		B	26.36		2,4-di-tert-butylphenol	96-76-4					Phenolic	1.44E+05	
170		B	26.42		α-bisabolol	72691-24-8						1.24E+05	
	49	C		26.53					Piggy, Barnyard, Urinous				
171		B	26.96		7-methoxycoumarin	531-59-9				Balsamic, Sweet	Balsamic	3.15E+05	
172	50	A	27.62	27.63	Piperonal	120-57-0		4.79E-03	Potato, Resiny		Floral	6.10E+03	1.28E+06
173		B	27.86		Caryophyllene oxide	1139-30-6				Herb, Sweet, Spice	Woody	1.74E+07	
	51	C		27.98					Resiny, Potato, Roasted, **Characteristic**				
	52	C		29.22					Potato, Resiny				

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174		B	29.83		4-ethoxy-3-anisaldehyde	120-25-2					Vanilla	4.86E+04	
175	53	A	30.46	30.47	Dibutyl phthalate	84-74-2			Potato, Resiny		Bland	1.61E+04	
176		B	31.47		Hexestrol	84-16-2						1.11E+06	
177		B	31.49		p-tert-butylphenol	98-54-4					Leathery	5.84E+05	
178		B	31.79		2,6-diethylpyrazine	13067-27-1	6.00E-03				Nutty, Hazelnut	1.96E+05	

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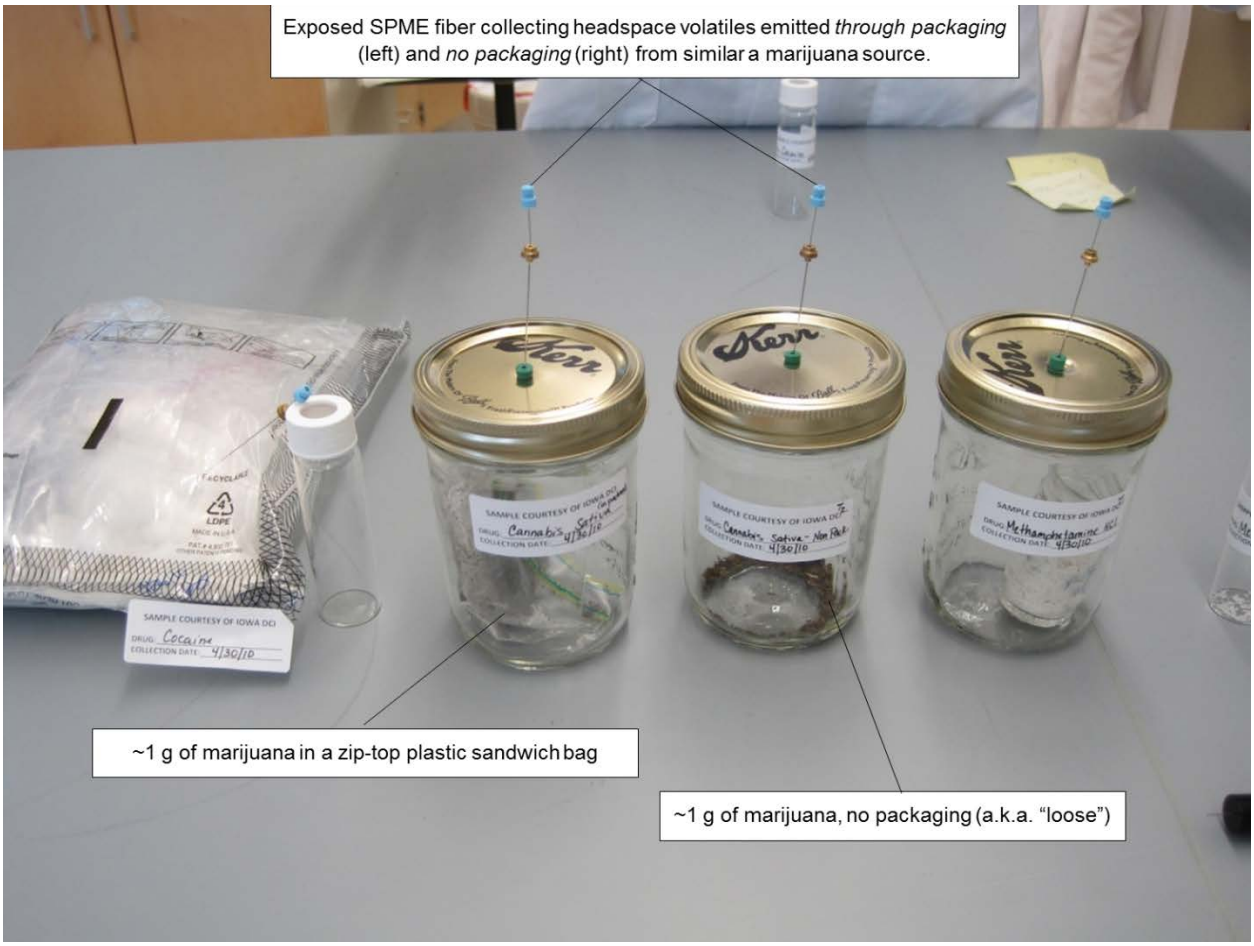
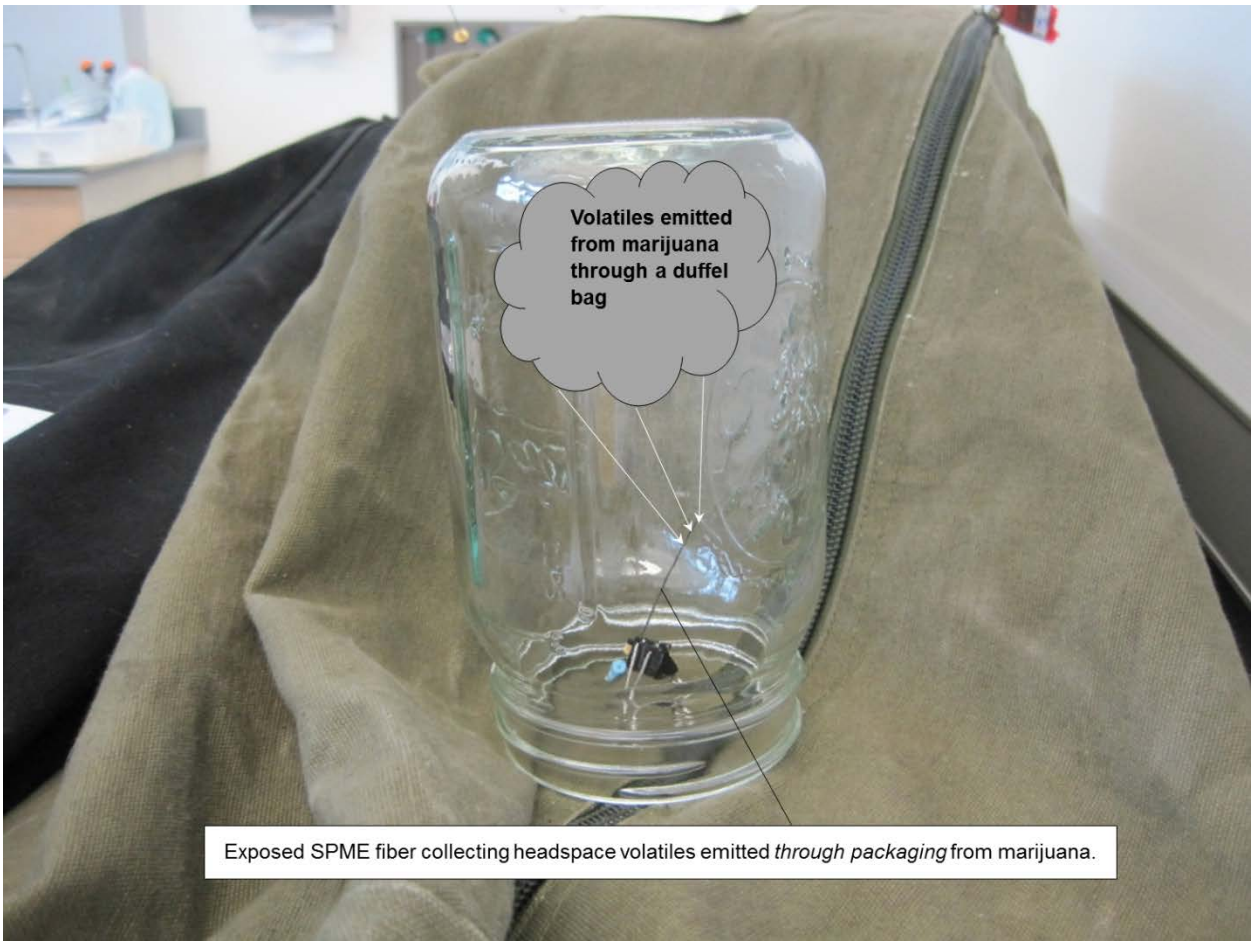
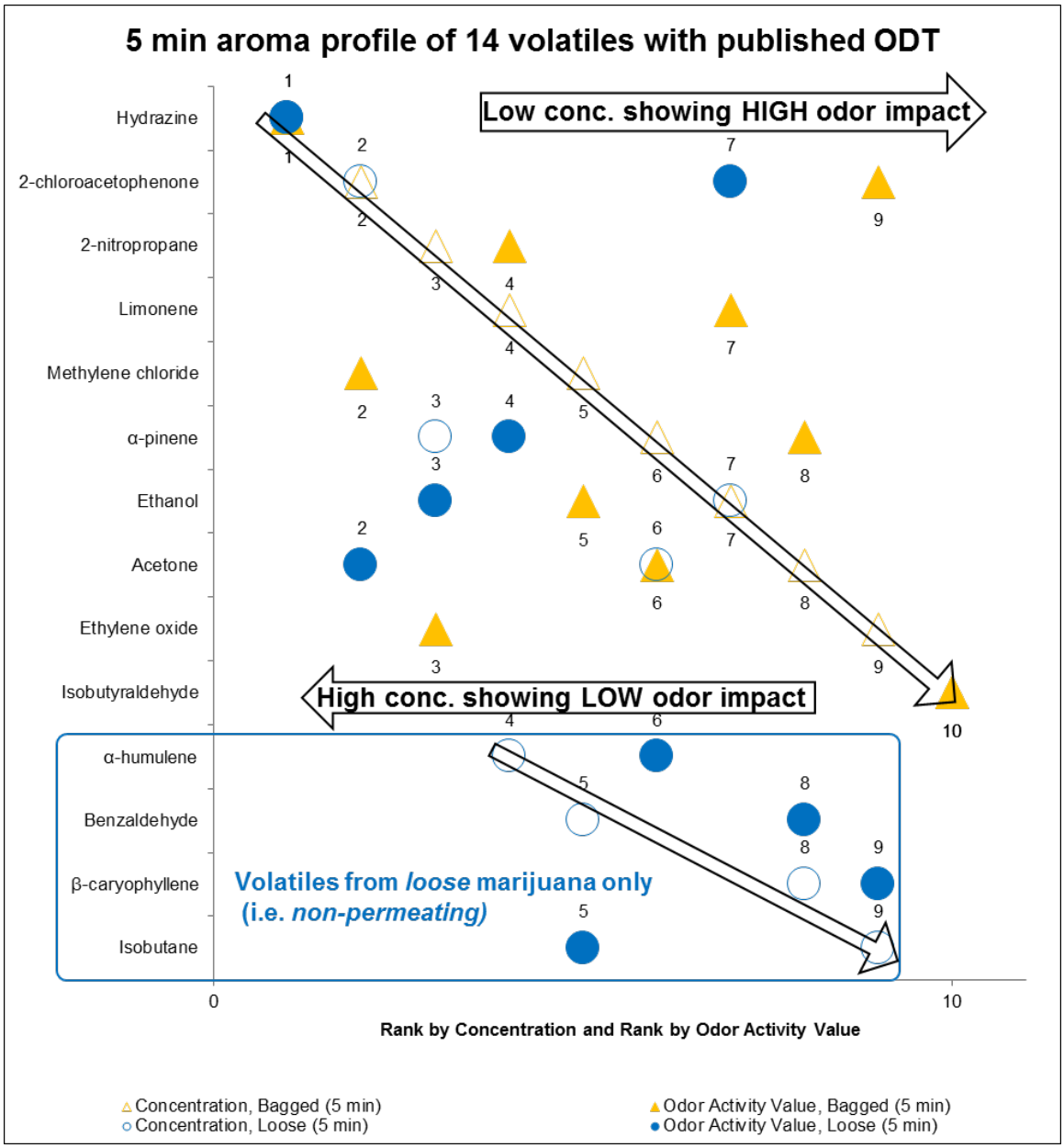


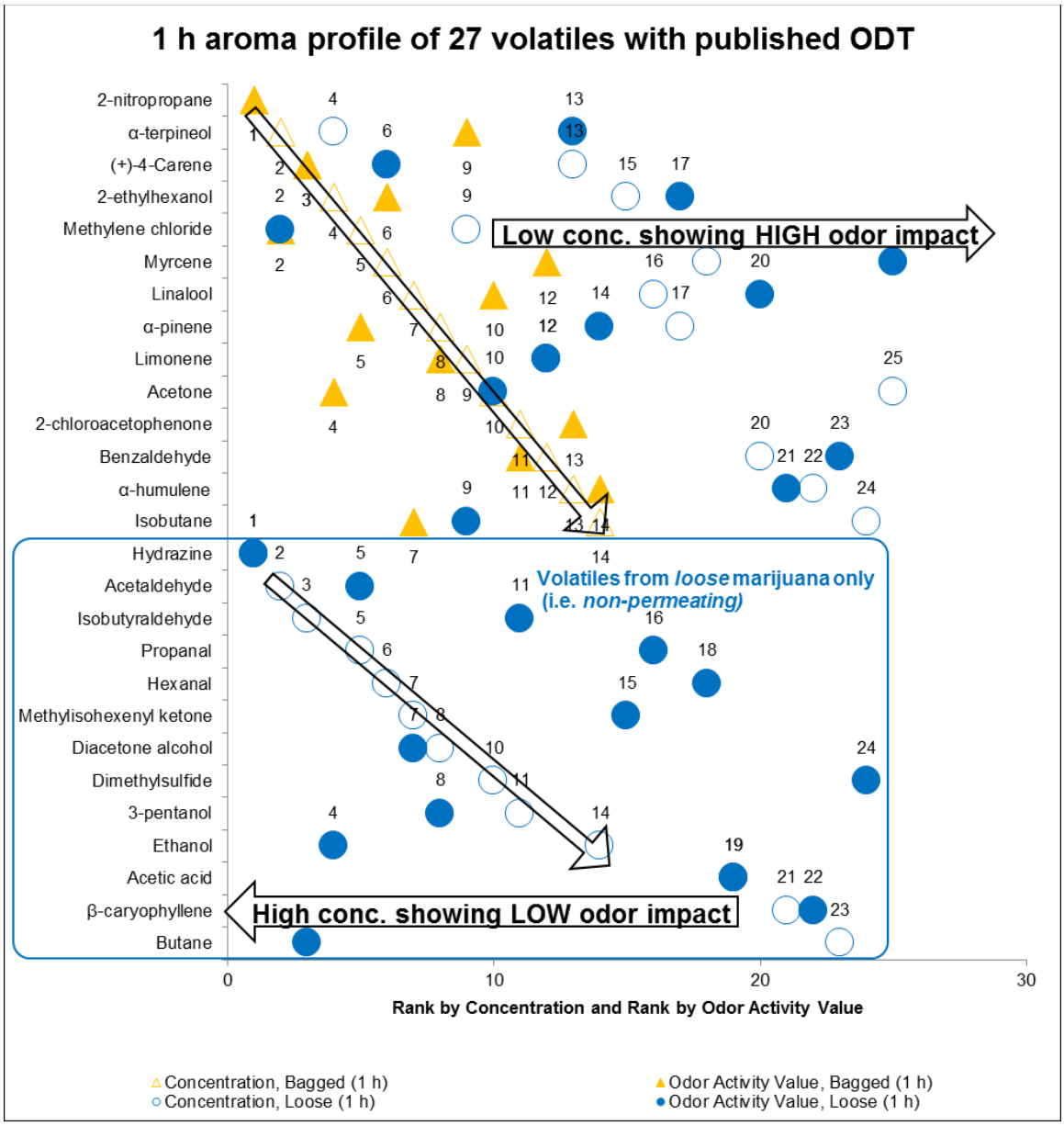
SI Figure 1. Static headspace sampling of VOCs emitted at room temperature from illegal street drugs. (Samples from left to right) The SPME fiber is exposed and sampling in between the evidence bag and original packaging of cocaine. ~1 gram of air-dried marijuana in a zip-top plastic sandwich bag. ~1 gram of air-dried marijuana, loose in the jar. Methamphetamine in a beaker. Holes were predrilled into the metal mason jar lids, and fitted with a half-hole septa as the SPME sampling port. All jars, lids, rings, and septa were pre-cleaned and baked out in 110 °C oven overnight to desorb interfering VOCs. Pre-conditioned SPME fibers were pre-cleaned prior to sampling by desorbing in a 270 °C GC injection port under flow of nitrogen, retracted, and wrapped in aluminum foil for transport. Sample loaded fibers were transported back to the lab wrapped in clean foil, placed in a clean jar with intact metal lid, and kept in a cooler with reusable ice packs.



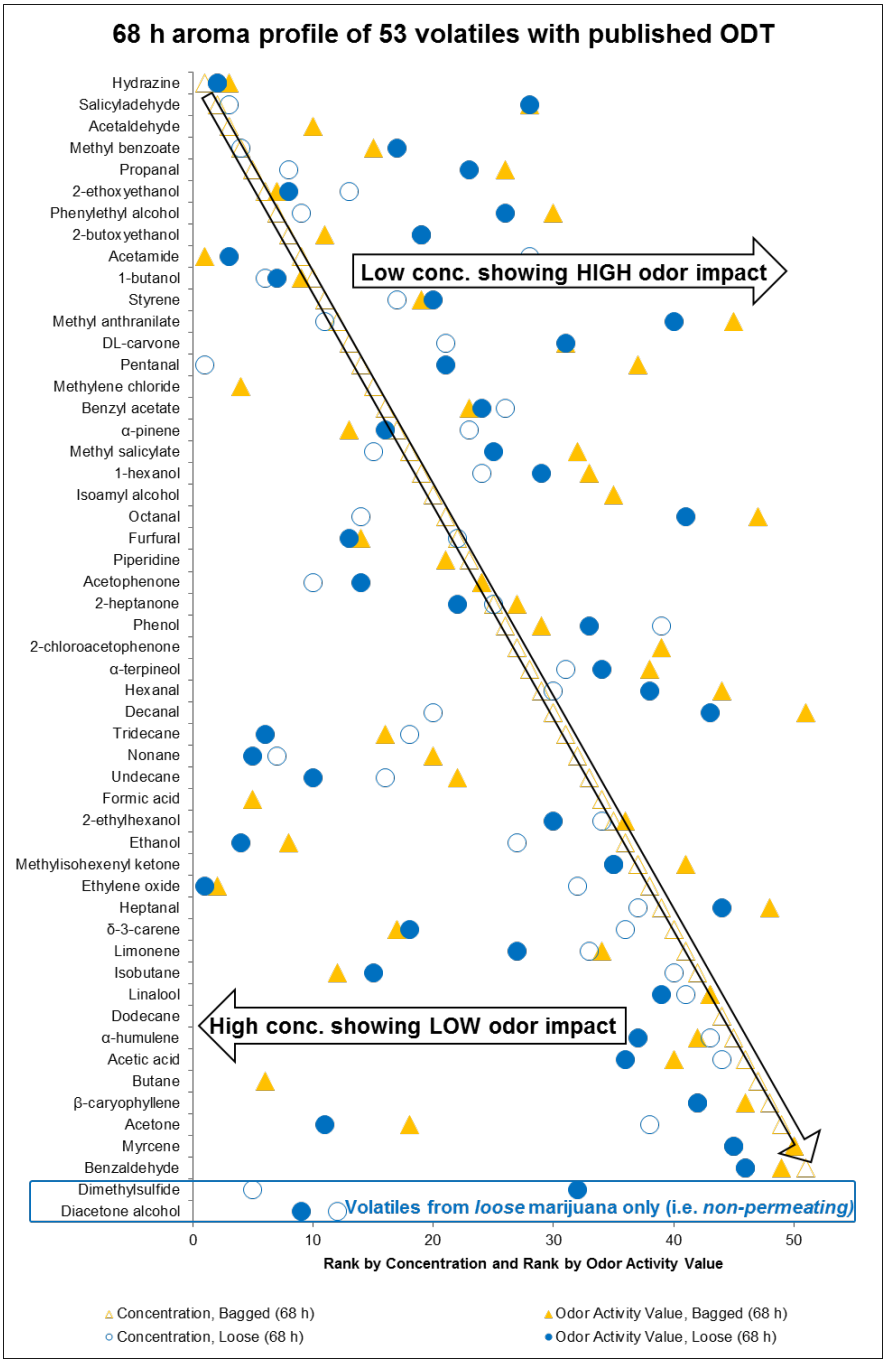
SI Figure 2. Static headspace sampling of VOC at room temperature from marijuana emitted though a duffel bag. A US military-style duffel bag containg ~50 kg of marijuana was siezed and tagged as evidence. The SPME fiber was exposed and propped up by a metal binder clip, inside an over-turned, pre-cleaned 16 oz glass mason jar. This ad hoc apparatus created a headspace sampling chamber to collect VOC emitted from the marijuana and through the duffel bag over a period of 68 hours. The fiber was transported back to the lab for analysis as described in the caption of SI Figure 1.



SI Figure 3. Dot plot illustrating hierarchy of volatiles emitted from marijuana using concentration and calculated odor activity value from published ODT at 5 min. Open markers represent the rank of the volatile based on concentration. Closed markers represent the rank of the volatile based on odor activity value. Horizontal axis reads from left to right, indicating least to most concentrated/odor active rank. Rank number is provided above and below markers for ease of reading. The general inference is a shift in rank based on odor activity value. Compounds with low detection thresholds tend to rank higher in OAV than rank of concentration in headspace, a relationship shown by Eq. 1. Blue box-outlined markers indicate volatiles detected in unpackaged marijuana and not detected by through-package sampling.



SI Figure 4. Dot plot illustrating hierarchy of volatiles emitted from marijuana using concentration and calculated odor activity value from published ODT at 1 h. Open markers represent the rank of the volatile based on concentration. Closed markers represent the rank of the volatile based on odor activity value. Horizontal axis reads from left to right, indicating least to most concentrated/odor active rank. Rank number is provided above and below markers for ease of reading. The general inference is a shift in rank based on odor activity value. Compounds with low detection thresholds tend to rank higher in OAV than rank of concentration in headspace, a relationship shown by Eq. 1. Blue box-outlined markers indicate volatiles detected in unpackaged marijuana and not detected by through-package sampling.



SI Figure 5. Dot plot illustrating hierarchy of volatiles emitted from marijuana using concentration and calculated odor activity value from published ODT at 68 h. Open markers represent the rank of the volatile based on concentration. Closed markers represent the rank of the volatile based on odor activity value. Horizontal axis reads from left to right, indicating least to most concentrated/odor active rank. Rank number is provided above and below markers for ease of reading. The general inference is a shift in rank based on odor activity value. Compounds with low detection thresholds tend to rank higher in OAV than rank of concentration in headspace, a relationship shown by Eq. 1. Blue box-outlined markers indicate volatiles detected in unpackaged marijuana and not detected by through-package sampling.

REFERENCES

1 Payton v. New York, 445 U.S. 573 (1980)

2 Maryland v. Macon, 472 U.S. 463 (1985)

3 Davis v. United States, 328 U.S. 582 (1946)

4 United States v. Robinson, 414 U.S. 218 (1973)

5 New Jersey v. TLO, 469, U.S. 325 (1985)

6 Arizona v. Gant, 129 S. Ct. 1710 (2009)

7 Illinois v. Cabales, 543 U.S. 405 (2005)

8 United States of America v. Harris, 846 F. Supp. 121 (1994)

9 Kabir, A., Holness, H., Furton, K. G. & Almirall, J. R. Recent advances in micro-sample preparation with forensic applications. *Trac-Trends in Analytical Chemistry* **45**, 264-279, doi:10.1016/j.trac.2012.11.013 (2013).

10 Furton, K. G., Wang, J., Hsu, Y. L., Walton, J. & Almirall, J. R. The use of solid-phase microextraction-gas chromatography in forensic analysis. *Journal of Chromatographic Science* **38**, 297-306 (2000).

11 Furton, K. G. & Myers, L. J. The scientific foundation and efficacy of the use of canines as chemical detectors for explosives. *Talanta* **54**, 487-500, doi:10.1016/s0039-9140(00)00546-4 (2001).

12 Kongshaug, K. E., Pedersen-Bjergaard, S., Rasmussen, K. E. & Krogh, M. Solid-phase microextraction/capillary gas chromatography for the profiling of confiscated ecstacy and amphetamine. *Chromatographia* **50**, 247-252, doi:10.1007/bf02490660 (1999).

13 Furton, K. G., Hsu, Y. L., Luo, T. Y., Norelus, A. & Rose, S. in *Meeting on Investigation and Forensic Science Technologies.* 41-46.

14 Hood, L. V. S. & Barry, G. T. Headspace volatiles of marijuana and hashish-gas-chromatographic analysis of samples of different geographic origin. *Journal of Chromatography* **166**, 499-506, doi:10.1016/s0021-9673(00)95633-4 (1978).

15 Ross, S. A. & ElSohly, M. A. The volatile oil composition of fresh and air-dried buds of Cannabis sativa. *Journal of Natural Products* **59**, 49-51, doi:10.1021/np960004a (1996).

16 Rothschild, M., Bergstrom, G. & Wangberg, S. A. Cannabis sativa: volatile compounds from pollen and entire male and female plants of two variants, Northern Lights and Hawaian Indica. *Botanical Journal of the Linnean Society* **147**, 387-397, doi:10.1111/j.1095-8339.2005.00417.x (2005).

17 Bertoli, A., Tozzi, S., Pistelli, L. & Angelini, L. G. Fibre hemp inflorescences: From crop-residues to essential oil production. *Industrial Crops and Products* **32**, 329-337, doi:10.1016/j.indcrop.2010.05.012 (2010).

18 Porto, C. d., Decorti, D., Natolino, A. & da Porto, C. Ultrasound-assisted extraction of volatile compounds from industrial Cannabis sativa L. inflorescences. *International Journal of Applied Research in Natural Products* **7**, 8-14 (2014).

19 Macias, M. S., Harper, R. J. & Furton, K. G. A comparison of real versus simulated contraband VOCs for reliable detector dog training utilizing SPME-GC-MS. *American Biotechnology Laboratory* **26**, 26-27 (2008).

20 Jezierski, T. et al. Efficacy of drug detection by fully-trained police dogs varies by breed, training level, type of drug and search environment. *Forensic Science International* **237**, 112-118, doi:10.1016/j.forsciint.2014.01.013 (2014).

21 Lit, L., Schweitzer, J. & Oberbauer, A. Handler beliefs affect scent detection dog outcomes. *Animal Cognition* **14**, 387-394 (2011).

22 Doty, R. L., Wudarski, T., Marshall, D. A. & Hastings, L. Marijuana odor perception: Studies modeled from probable cause cases. *Law and Human Behavior* **28**, 223-233, doi:10.1023/B:LAHU.0000022324.13389.ea (2004).

23 Acree, T. E. & Arn, H. Flavornet and human odor space. http://flavornet.org/flavornet.html (2004). Accessed September 8, 2014

24 The Good Scents Company Information System. http://www.thegoodscentscompany.com/index.html# (1994). Accessed August 8, 2014.

25 Mottram, R. LRI & Odour Database. www.odour.org.uk/index.html (2006). Accessed August 1, 2014.

26 M. Devos, F. P., J. Rouault, P. Laffort, L.J. Van Gemert. Standardized Human Olfactory Thresholds. (IRL Press at Oxford Press, 1990).

CHAPTER 4. THE RELATIONSHIP BETWEEN CHEMICAL CONCENTRATION AND ODOR ACTIVITY VALUE EXPLAINS THE INCONSISTENCY IN MAKING A COMPREHENSIVE SURROGATE SCENT TRAINING TOOL REPRESENTATIVE OF ILLICIT DRUGS

Modified from a paper submitted to *Forensic Science International*

Somchai Rice [a, b], Jacek A. Koziel [b, *]

Abstract

This report highlights the importance of odor in the olfactory identification of marijuana, cocaine, and heroin. There are small amounts of highly odorous compounds present in headspace of these drugs, with very low odor detection thresholds, that are more likely responsible for contributing to the overall odor of these drugs. Previous reports of the most abundant compounds in headspace can mislead researchers when dealing with odor of these compounds. Surrogate scent formulations, therefore, need to improve matching the odor impact of key compounds and not just the chemical abundance of compounds detected. When manufacturing these compounds, utmost care needs to be taken to ensure contaminating odors are not accidentally added. It is shown that if the odor detection threshold is very small, only a small amount of the contaminant is enough to affect the overall odor of the surrogate training tool.

The use of solid phase microextraction allowed volatile organic compounds in headspace to be extracted and pre-concentrated on site, and analyzed by multidimensional gas chromatography – mass spectrometry – olfactometry. Use of this state of the art instrumentation allowed for further separation of odorous compounds and simultaneous detection by human nose to further elucidate the separate odor parts

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that make up the whole of the total aroma of these drugs. The concept of odor activity value, then, is useful to researchers without such instrumentation. Odor activity values can be calculated from published odor detection thresholds. More research is warranted to expand the database, and determine odor detection thresholds for compounds of interest.

Introduction

Identification of odors has been widely explored with differing theories as to the mechanism of action. Odor character of 281 compounds in water were characterized as early as 1988 [1]. Yoshii, Yamada, et al. investigated 62 structurally rigid compounds and characterized the corresponding odor strengths [2]. Steric and electrostatic properties of compounds have been used to determine the odor characteristic as perceived by human olfaction [3]. It has been suggested that structure-activity can be used to predict odor detection thresholds (ODT) [4]. ODT is the lowest concentration at which 50% of the population can detect an odorant [5]. Odor activity value (OAV) is calculated as the ratio of the concentration to the ODT, in dimensionless units [6]. Despite studies spanning over 30 years on odor, odor character, and mechanisms of detection, there is still no consensus on perception of odor.

ODT and OAV have been used to characterize the characteristic odors of many sample matrices. For example, highly odorous compounds have been identified in essential oils [7], young Riesling and non-Riesling wines [8], and even emissions from animal buildings [9]. It has been shown that ODTs decrease with increase in carbon chain length, from propanal to octanal, but sharply increased with nonanal [10]. Although

odor intensity and odorant concentration has been directly correlated under intense sources [11], highly impactful odor compounds are found in smaller concentration and can easily be overlooked [12].

There has been a long standing interest on the subject of odor and its application to forensics. Pig carcasses have been evaluated for volatile organic compounds (VOC) generated by decomposition; pig carcasses are the current surrogates for human decomposition studies [13]. It has been shown that cadaver detector dogs were able to detect human remains 667 days post removal of the body, although the chemical composition of the emitted VOCs were not investigated [14]. Seasoned bloodhounds can track and discriminate between two individuals [15] and human remains in the environment even when an object is not even touched [16]. An electronic nose was used to differentiate cannabis and tobacco smoking subjects by human body odor [17]. Research has been focused on the VOCs emitted, and not on the odor character, ODTs, or OAVs of key odorous compounds.

Researchers know that these forensic samples emit chemical odor signatures. When surrogate formulations are made to mimic real field samples, and tested using odor detection dogs, they fail to illicit the same response as the actual sample. Cadaver pseudo scent was evaluated [18], composition C-4 volatiles investigated [19], and narcotic scents have been studied [20, 21]. There is a need for reliable training aids for detection of drugs, cadavers, and explosives by smell; the previously mentioned studies show poor efficacy. The key to creating a comprehensive odor mimic could be in creating a surrogate with matching odor activity values to the actual sample. This has been

demonstrated in a model rice wine made by mixing aroma compounds with OAVs > 1 in an odorless matrix, showing similarity to the aroma of the original rice wine [22].

The objective of this study was to compare odorous VOCs emitted from illicit drug samples of marijuana, cocaine, and heroin to their commercially available surrogate smell formulations using simultaneous sensory and chemical analyses. The working hypothesis is that the training aids do not smell like the real drugs. This is due to several factors: (1) absence of some key, high impact odorants and (2) surrogate smell is overloaded with a few compounds of lesser odor/aroma importance that are selected solely as a match to major chemical components. A mathematical example would be to compare the odor activity values of nerol (ODT = 0.3 ppm) [23] and α-pinene [24] (ODT = 0.69 ppm), both found in marijuana [25]. OAV is calculated as the ratio of concentration to ODT, with assumed equal concentrations of the compounds present in headspace (1 ppm), the odor activity value of nerol is the dimensionless unit 3.33 and the odor activity value of α-pinene is 1.45. Nerol, at the same concentration of α-pinene, is a *more* odor active compound (larger calculated OAV) and therefore is likely to make a more important contribution to the overall characteristic aroma of marijuana. In other words, it would only take 0.44 ppm of nerol to equal the odor impact of 1 ppm α-pinene. This is a paradigm shifting approach to odor detection in the field of forensic sciences. Novelty of SPME, MDGC-MS-human olfactometry. To date, this is the first report of using simultaneous chemical and sensory analysis to evaluate surrogate training aids and real illicit drugs (marijuana, cocaine, and heroin).

Materials and methods

Aromas were characterized by human nose from volatiles emitted into the headspace of illicit marijuana, cocaine, and heroin. Various states of seizure were examined: 1) 50 kg of marijuana in a cloth military style duffel bag 2) 1g marijuana packaged in a plastic zip-top sandwich bag 3) 1 g old, desiccated marijuana with no packaging 4) plastic zip-top sandwich bag with 1 g marijuana removed 5) 1 g crack cocaine packaged as tear drops 6) 1 g cocaine adulterated with Levamisole 7) an 1 kg evidence pack containing cocaine 8) 1 g cocaine in a plastic bag, opened 9) 1 g heroin seized in 1997 10) 1 g heroin seized in 2010.

Sigma Pseudo™ Narcotic Scent Marijuana formulation (Fluka, #P7309), Sigma Pseudo™ Narcotic Scent Cocaine formulation (Fluka, #P2423), and Sigma Pseudo™ Narcotic Scent Heroin formulation (Fluka, #P2548) were purchased from Sigma-Aldrich (St. Louis, MO). Table 3 provides a key to the various samples taken, how they are referred to in the text, relevant matrix conditions, and the reference codes for SI Table 9, SI Table 10, and SI Table 11.

Table 3. Key of all samples analyzed in this study

In text reference	Matrix condition	Code
	Marijuana	
Duffel bag sample	~50 kg of marijuana in duffel bag	A1
Duffel bag sample	~50 kg of marijuana in duffel bag	A2
Duffel bag sample	~50 kg of marijuana in duffel bag + lab air	A3
1 g sample	~1 g of marijuana in plastic bag	A4
1 g sample	~1 g of Marijuana in Plastic Bag	A5
1 g sample	~1 g of Marijuana loose in jar	A6
1 g sample	~1 g of Marijuana loose in jar	A7
Residual sample	Empty marijuana sample jar, ~1 g of marijuana removed	B1
Residual sample	Empty marijuana sample jar, ~1 g of marijuana removed	B2
Residual sample	Empty Plastic Bag in jar, ~1 g of marijuana removed	B3
Residual sample	Empty Plastic Bag in jar, ~1 g of marijuana removed	B4
Surrogate sample	~1 g of Marijuana Pseudo Scent	C1

Table 3 continued…

In text reference	Matrix condition	Code
Surrogate sample	~1 g of Marijuana Pseudo Scent	C2
Surrogate sample	~1 g of Marijuana Pseudo Scent	C3
	Cocaine	
1 g sample	~1 g of Cocaine- Crack in teardrops	D1
1 g sample	~1 g of Cocaine with Levamisole	D2
Evidence pack	Cocaine- through evidence pack	D3
1 g sample	~1 g of Cocaine, bag opened, in jar	D4
1 g sample	~1 g of Cocaine, bag opened, in jar	D5
1 g sample	~1 g of Cocaine Pseudo Scent	E1
	Heroin	
1 g sample	~1 g of Heroin (1997)	F1
1 g sample	~1 g of Heroin	F2
Surrogate sample	~1 g of Heroin Pseudo Scent	G1

Sampling conditions, instrumental parameters, along with chemical and sensory data acquisition are similar to what is outlined in Materials and Methods of Chapter 2. The exception is headspace-SPME extraction was carried out for 1 h at ambient temperature.

Results and discussion

1. Marijuana odor

A. Real marijuana vs. surrogate marijuana scent

Figure 5 highlights the importance of odor impact (represented with OAVs), where concentration in headspace is not directly proportional to odor impact. When concentration of volatiles emitted from 1 g of real marijuana were compared to volatiles emitted from 1 g Sigma Pseudo™ Narcotic Scent Marijuana formulation, under identical sampling and analysis conditions, the following chemical groups were absent or underrepresented in the surrogate scent: acids, halogenates, hydrocarbons, ketones, and sulfur containing VOCs. When compared to 1 g of real marijuana, the following

chemical groups were more abundant in headspace of surrogate scent: alcohols, aldehydes, aromatics, esters, ethers, nitrogen containing and phenols. The distance between the markers is proportional to the knowledge of odor impact; large distances signify a higher degree of knowledge, whereas small to zero difference signifies little known or no published ODTs for the compound. Using this metric, current knowledge on odor impact is strongest regarding esters and knowledge is weak in acids, aldehydes, nitrogen containing compounds and phenols. A great distance between solid black line and round markers indicates a large discrepancy between odor impact and concentration in headspace of these compounds. An absent solid black line along a radial arm indicates compounds with no OAVs calculated (i.e. acids, halogenates, and nitrogen containing), either because of no available published ODTs (i.e., acids and nitrogen containing) or were not detected, ND, (i.e., halogenates and sulfur containing). None of the phenols detected in 1 g real marijuana by MS had published ODTs, and no OAV comparison is possible, thus OAV data shown are absolute values and are not scaled relative to 1 g real marijuana (100%), at approximately 3,800,000%. Based on this new information, in order to make a more representative recipe that targets odor of 1 g marijuana, one approach would be to add or reduce chemicals based on their calculated odor activity values to match the odor target (i.e., line up the solid line and dashed lines). Rank of volatiles by odor impact, highest to lowest, for the odor of 1 g of marijuana are aromatics, alcohols, ketones, esters, and phenols. For full details including identification, significant ions by MS, % spectral match by AMDIS, CAS, published odor descriptors, published ODTs, and calculated OAVs of the chemicals

detected in headspace of all marijuana samples and surrogate scent marijuana formulation, please see SI Table 9, page 130.

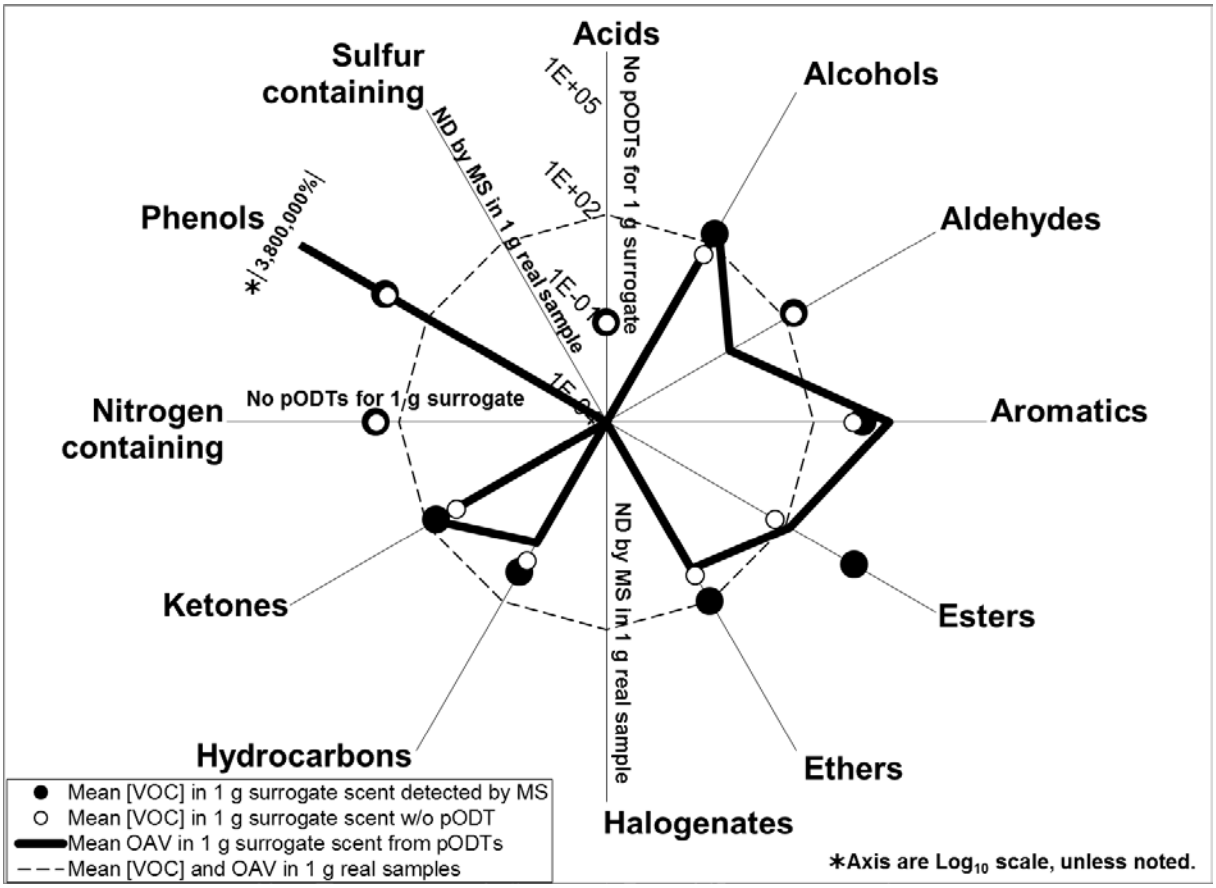

Figure 5. Comparison of VOC concentrations and odor activity values (OAVs) calculated from published odor detection values (ODTs) emitted from 1 g of real marijuana (represented as a reference dashed line at 100%) with 1 g Sigma Pseudo™ Narcotic Scent Marijuana formulation. The majority of chemical compound groups are mismatched with the target chemical content and odor impact, i.e., the position of solid black markers and solid line do not line up along the black dashed line, which would indicate 100% odor and chemical match on a % Log_{10} scale. Solid black markers indicate mean concentration of compounds detected by MS. White filled markers indicate the percentage of missing information in the form of no published ODTs available, i.e., the distance between these two markers indicates the level of current knowledge in odor impact of these compounds. An absent solid black line along a radial arm indicates compounds with no OAVs calculated, either because of no available published ODTs. None of the phenols detected in 1 g real marijuana by MS had published ODTs, and no OAV comparison is possible.

B. Effects of quantity of sample on marijuana odor perception

It is reasonable to hypothesize that the amount of sample present will affect the amount of volatiles emitted, thus odors will be different between 1 g of marijuana and 50 kg of marijuana, i.e., more sample mass leads to higher concentration of volatiles emitted. Figure 6 illustrates the differences in concentration of volatiles emitted and associated odor impact of these volatiles between 1 g and 50 kg of marijuana. Acids, alcohols, ketones, and sulfur containing volatiles in headspace were detected by MS at a lower rate in 50 kg marijuana samples than 1 g marijuana samples. Factors that could affect this are affinity of the compounds to Carboxen/PDMS SPME coating, displacement by more competitively binding volatiles, or rates of diffusion of certain volatiles through packaging and were not explored in this study. All other chemical groups present in headspace of 50 kg of marijuana were at or exceeded the concentration of volatiles present in 1 g marijuana headspace. All aldehydes and sulfur containing volatiles had published ODTs. In contrast, all other chemical groups are missing published ODTs to calculate accurate OAVs. Even though concentration of esters in 50 kg of marijuana was two orders of magnitude higher than 1 g samples of marijuana, the odor impact imparted by these compounds was 40% less than that of 1 g samples. Nitrogen containing compounds were doubled in 50 kg marijuana samples, but odor impact was two orders of magnitude higher than 1 g marijuana samples. As previously stated, no OAV comparison is possible for phenols relative to 1 g marijuana samples. Phenols were detected in headspace of 50 kg of marijuana, but no OAV was calculated due to unpublished ODTs. More work on establishing the missing ODTs for these compounds will further our understanding of forensic odor. Using current

information presented in this study, top volatile responsible for the odor of 50 kg of marijuana are nitrogen containing, aldehydes, hydrocarbons and aromatics relative to 1 g marijuana samples.

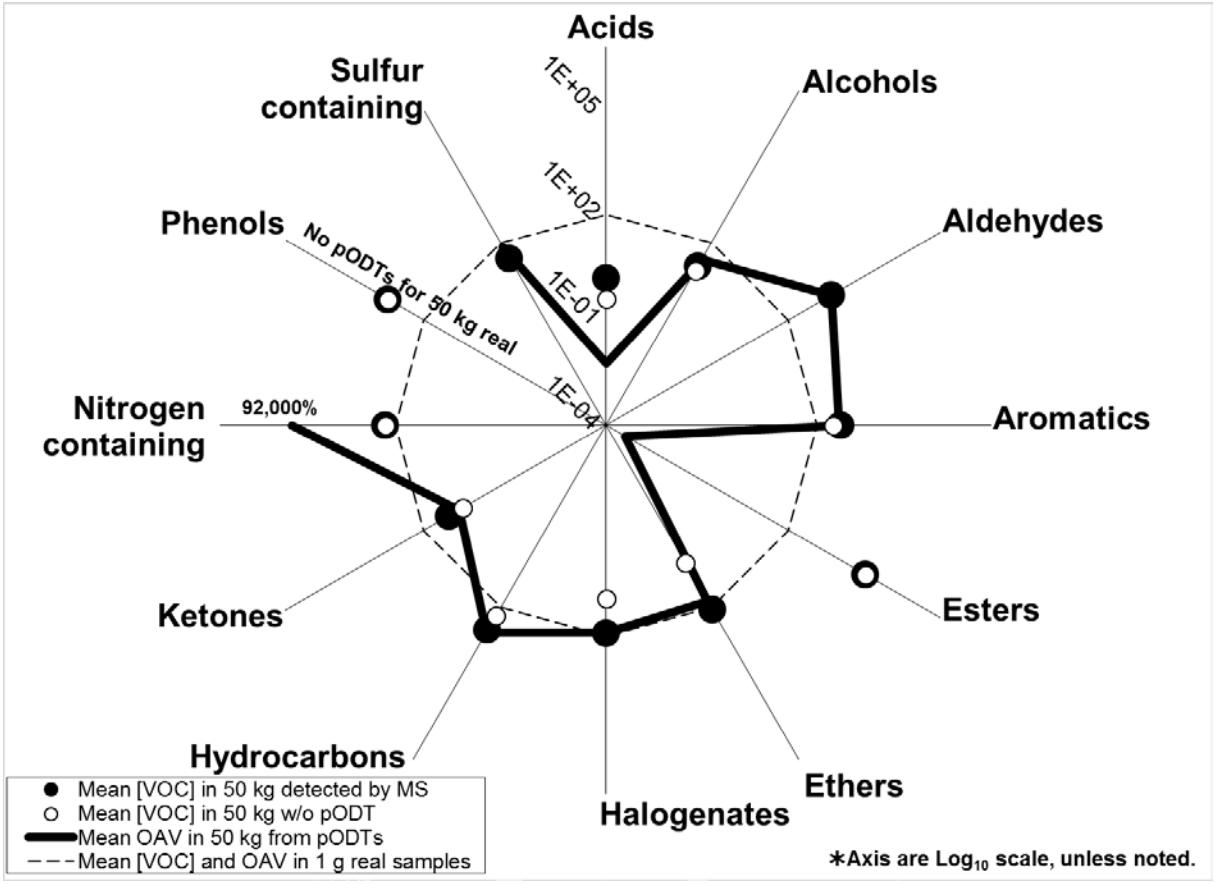

Figure 6. Comparison of VOC concentrations and odor activity values (OAVs) calculated from published odor detection values (ODTs) emitted from 1 g of real marijuana (represented as a reference dashed line at 100%) with 50 kg of marijuana in a duffel bag. The majority of chemical compound groups are mismatched with the target chemical content and odor impact, i.e., the position of solid black markers and solid line do not line up along the black dashed line, which would indicate 100% odor and chemical match on a % Log_{10} scale. Solid black markers indicate mean concentration of compounds detected by MS. White filled markers indicate the percentage of missing information in the form of no published ODTs available, i.e., the distance between these two markers indicates the level of current knowledge in odor impact of these compounds. An absent solid black line along a radial arm indicates compounds with no OAVs calculated, either because of no available published ODTs. None of the phenols detected in 1 g real marijuana by MS had published ODTs, and no OAV comparison is possible.

C. Comparing odor profiles by OAVs

The odor profiles, based on calculated OAVs, of 1 g and 50 kg real marijuana and 1 g surrogate marijuana scent were compared. Compounds most important to the total odor of 1 g marijuana (most to least impact) are aromatics, acids, ketones, hydrocarbons, alcohols, sulfur containing, esters, ethers, halogenated and nitrogen compounds. The compounds most important to the total odor of marijuana residue from a plastic bag are hydrocarbons, aromatics, nitrogen containing, ketones, aldehydes, acids, alcohols, phenols, ethers, halogenated and esters. Compounds most impactful on the total odor of 50 kg of marijuana in a duffel bag are aromatics, aldehydes, hydrocarbons, sulfur containing, alcohols, ketones, nitrogen containing, ethers, halogenated, acids, and esters. Compounds most impactful on the total odor of 1 g Sigma Pseudo™ Narcotic Scent Marijuana formulation are aromatics, alcohols, ketones, esters, phenols, hydrocarbons, aldehydes, and ethers. Halogenated and sulfur containing volatiles were not detected in the surrogate scent formulation, while acids and nitrogen containing volatiles did not have published ODTs to calculate OAVs. Figure 7 illustrates how 1 g Sigma Pseudo™ Narcotic Scent Marijuana formulation is not a representative odor mimic for the types of illicit marijuana sampled in Table 3, i.e., the solid black line is not congruent with any of the other lines. More importantly, since none of the lines are congruent, this information suggests that a single surrogate scent formulation would not be appropriate to use as a training tool to mimic the odor of marijuana in various packaging and various masses found in the field of forensics.

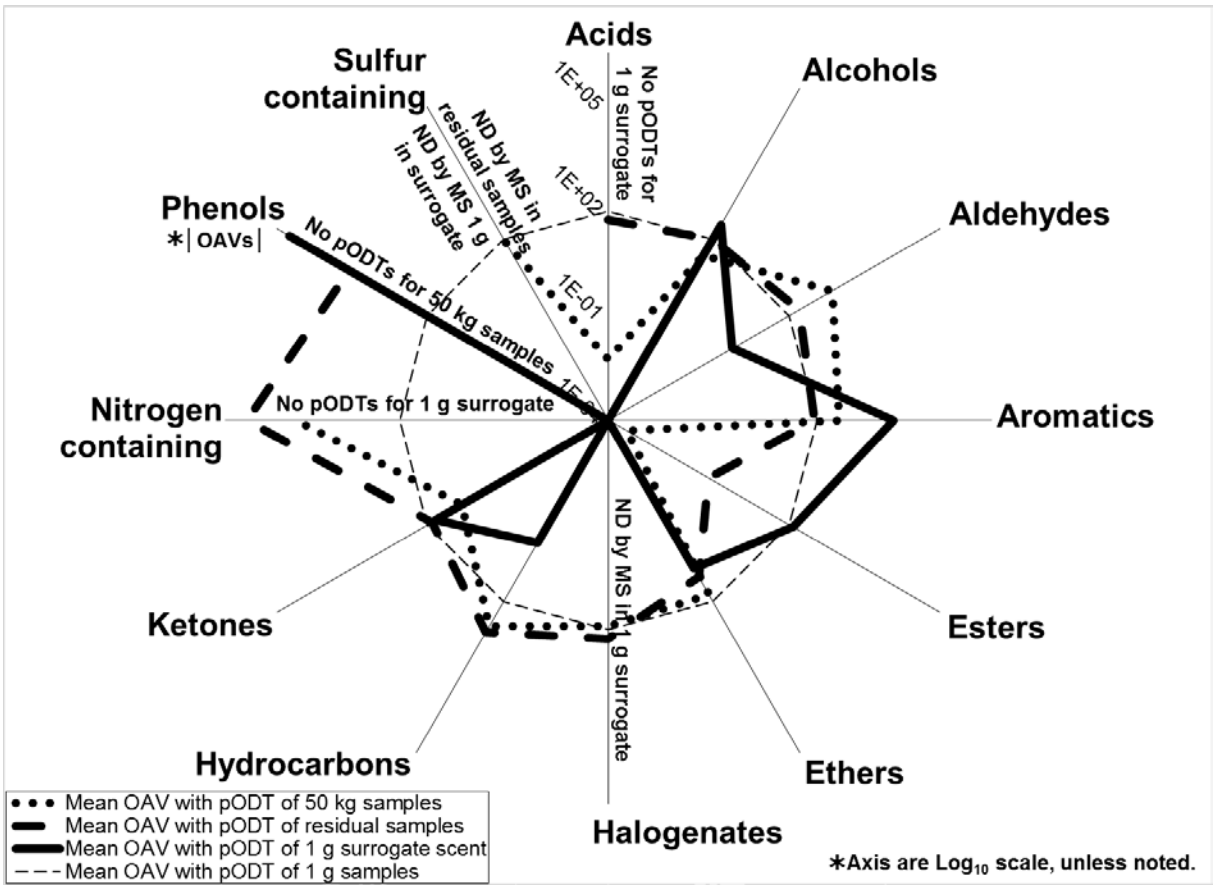

Figure 7. Marijuana odor is not a one-size-fits-all recipe for all states of seizure. A comparison of calculated odor activity values (OAVs) with published odor detection values (ODTs) emitted from 1 g of real marijuana (represented as a reference dashed line at 100%) with 50 kg marijuana in a duffel bag and 1 g Sigma Pseudo™ Narcotic Scent Marijuana formulation is shown. The majority of chemical compound groups are mismatched with the odor impact, i.e., the position of all the lines do not match up, which would indicate 100% odor match on a % Log_{10} scale. None of the **Phenols detected in 1 g real marijuana by MS had published ODTs, and no OAV comparison is possible, thus all OAVs shown are an absolute value of calculated OAV for surrogate scent and not scaled relative to 1 g real marijuana (100%). There were no published ODTs available for calculation of OAVs for acids and nitrogen containing compounds in surrogate scent, or phenols in duffel bag samples. Compounds were not detected by MS, thus no OAVs were calculated for halogenates and sulfur containing compounds in surrogate scent, and sulfur containing compounds in residual marijuana samples.

D. Simultaneous chemical and sensory analysis of marijuana

Figure 8 is an aromagram depicting the odor of marijuana (1 g) residue from a plastic bag and 1 g Sigma Pseudo™ Narcotic Scent Marijuana as detected by human nose. Note that the peaks with maximum height (i.e., intensity) do not elute at the same

retention time between the two samples indicating the most intense peaks cannot be the same compounds. The descriptor “characteristic” is used to describe the aroma that represents the overall scent of marijuana. There circled peaks (i.e., aroma events) detected by human nose show the inconsistencies that need to be remedied for an identical odor mimic, i.e., as detected by law enforcement canines, explaining why current surrogate formulations are not detected as real drug. Full details on odor description, hedonic tone, intensity, and retention time for each peak are given in Table 4 and Table 5.

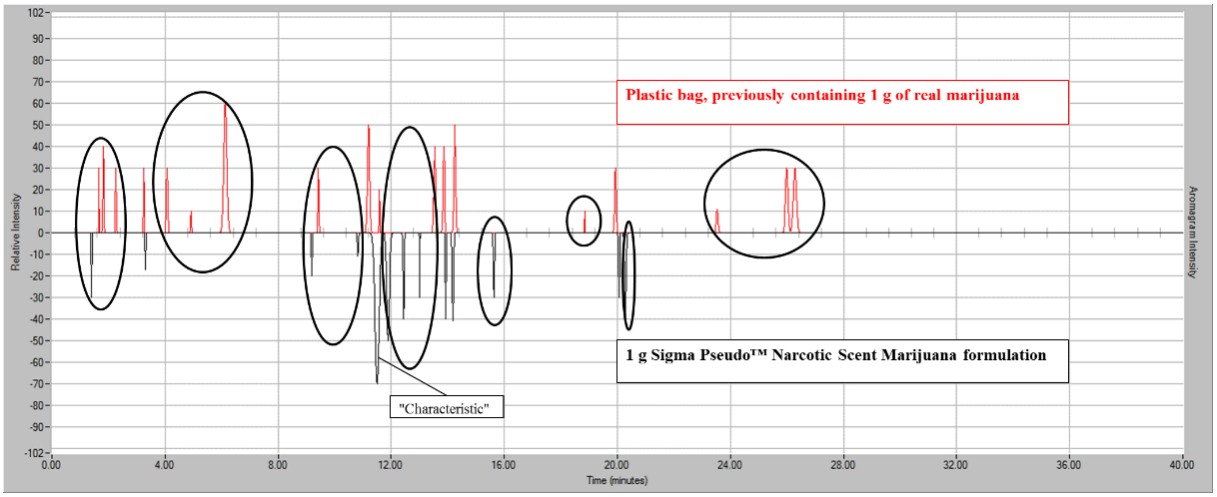

Figure 8. Example of aromagrams of 1 g Sigma Pseudo™ Narcotic Scent Marijuana formulation vs. residual marijuana odor emitted from a plastic bag, previously containing 1 g of real marijuana. Overlay of aromagrams generated with olfactometry data of Sigma Pseudo™ Narcotic Scent Marijuana formulation (inverted black signal, "C3" from Table 3, aroma details in Table 4 and residual marijuana odor emitted from a plastic bag previously containing 1 g of illicit marijuana (red signal, B4 of Table 3, aroma details in Table 5). “Characteristic” descriptor is used to tag an odor component that represents the overall aroma of the sample (i.e. typical smell of marijuana).

Figure 8 is an example of a typical overlay of TIC with aromagram, depicting the simultaneous chemical (red signal) and sensory analysis (black signal), respectively.

For the lot of Sigma Pseudo™ Narcotic Scent Marijuana formulation analyzed in this study, the ingredients listed in the material safety data sheets are pyrogenic colloidal silica (1%), cellulose (98.5%), butane-2, 3-diol (0.4%), and p-mentha-1, 2-diene (0.1%). Of these 4 ingredients, p-mentha-1, 4-diene (CAS 99-85-4, γ-terpinene, retention time 11.79 min, SI Table 9) was detected by the previously described method, and labeled by human panelist as “solvent, gasoline, mint”. Previously published odor characteristics of γ-terpinene are reported as “gasoline, turpentine”. Aroma event #5 (zoomed box) was flagged by the panelist as a characteristic aroma of marijuana and identified as p-cymene (SI Table 9) and described as “mint, fruity, sweet, characteristic”. The authors cannot explain the presence other chemical or odor peaks detected in the figure. Possible sources can include accidental introduction of contaminating compounds into the production of this surrogate scent formula or certain ingredients were omitted from MSDS due to proprietary formulations, or certain odors were absorbed through packaging during storage. This analysis highlights how there might be more odors present in surrogate scent formulation than intended, leading to misidentification by odor in the case of drug detection canines. Full details of odor character, hedonic tone, and intensity are given in Table 4.

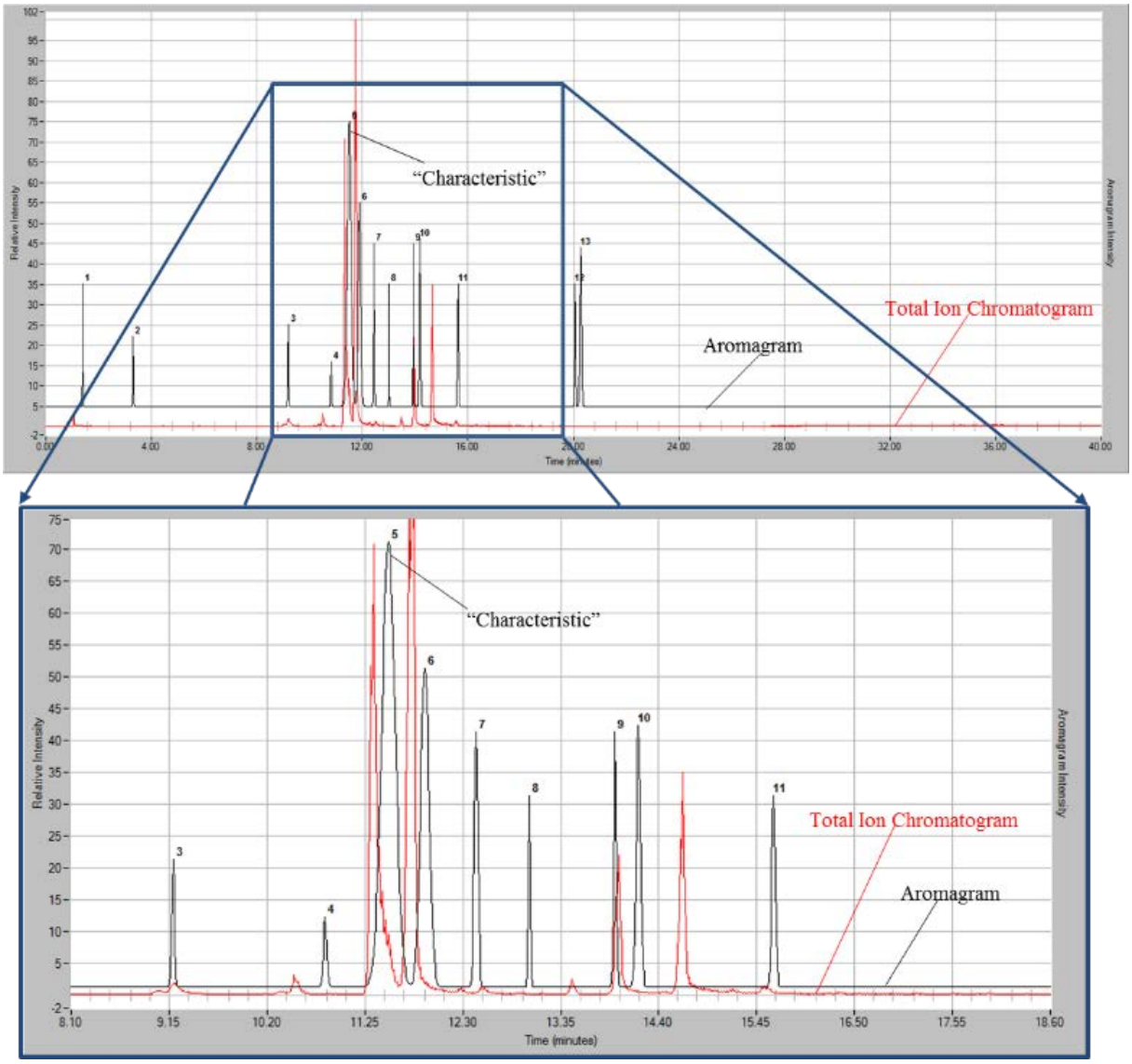

Figure 9. Example of a typical overlay of total ion chromatogram and aromagram of 1 g Sigma Pseudo™ Narcotic Scent Marijuana formulation. 1 h, static, extraction at room temperature of 1 g of Sigma Pseudo™ Narcotic Scent Marijuana formulation using Carboxen/PDMS SPME fiber. Chemical and aroma signals are generated simultaneously using a MD-GC-MS-O. Details on compounds in TIC are given in SI Table 9. Details on compounds in aromagram are provided in Table 4. Zoomed view shows mis/match of aromas detected and chemicals detected.

Table 4. Olfactometry results of sensory analysis of Marijuana Pseudo Scent

Event #	Descriptor	Hedonic Tone	Intensity	RT (min)	Width	Event Area
1	Solvent	Unpleasant -1	30	1.37	0.07	209
2	Buttery	Pleasant +1	17	3.28	0.07	118
3	Solvent	Unpleasant -1	20	9.15	0.08	159
4	Mushroom, Moldy	Neutral 0	11	10.77	0.1	109
5	Mint, Fruity, Sweet, **Characteristic**	Pleasant +2	70	11.30	0.4	2795
6	Solvent, Gasoline, Mint	Unpleasant -1	50	11.76	0.26	1297
7	Mint, Fruity	Pleasant +1	40	12.39	0.11	439
8	Foul	Unpleasant -1	30	12.99	0.05	149
9	Burnt, Burnt food	Unpleasant -2	40	13.90	0.08	319
10	Potato, Resiny	Neutral 0	41	14.12	0.13	532
11	Resiny	Unpleasant -1	30	15.58	0.11	329
12	Burnt food, Burnt	Unpleasant -1	30	20.02	0.1	299
13	Burnt, Burnt food	Unpleasant -1	39	20.20	0.17	661

Event # corresponds to numbered peaks in Figure 9. “Characteristic” descriptor is used to tag an odor component that represent the overall aroma of the sample (i.e. smell of marijuana). Hedonic tone is the overall pleasant or unpleasantness of the descriptor (range is Unpleasant -4, through 0, to Pleasant +4). Intensity is on a scale of 0-100, with 100 being most intense; intensity sets the peak height. RT = Retention Time. Width is defined as width at half-height of the Aromagram peak. Event area is a dimensionless value = Intensity x Width x 100, and is comparable to peak area counts generated with a mass selective detector.

Similar analysis of residual odor of marijuana from a plastic bag showed similar results. There are intense odors present when simultaneous chemical analysis by MS show zero or only small peaks. The most abundant chemical peak at 5.99 minutes was identified as hexanal, with panelist tagged descriptor and published odor character reported as grassy. This chemical was not found in 1 g surrogate scent marijuana formulation, but only found in 1 g of real marijuana, loose in a jar and residual marijuana odor. The next most intense odors (event # 9 and 13) have very small chemical signals, were not found in the AMDIS spectral library, but complete odor identification given in Table 5. ODT and odor characteristics for chemicals detected at the appropriate retention times are not known. Using the concept of odor activity values, one would expect that these compounds have low odor detection thresholds, allowing for detection by smell and not by MS.

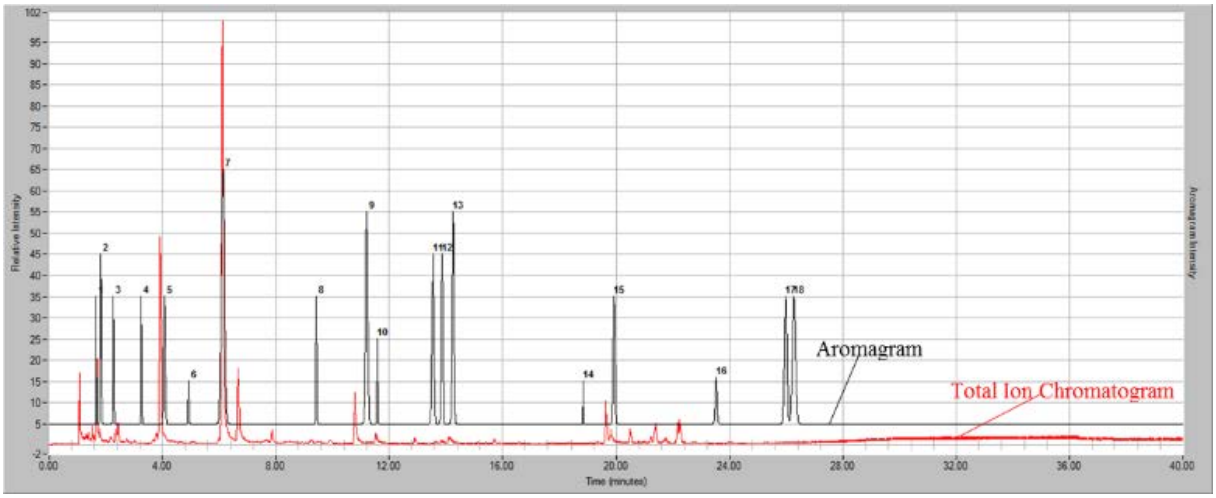

Figure 10. Example of typical overlay of total ion chromatogram and aromagram of residual marijuana in a plastic bag using MD-GC-MS-O (B4, Table 3). 1 h, static, room temperature extraction of VOCs emitted from a plastic bag previously containing 1 g of illicit marijuana, using Carboxen/PDMS SPME fiber. Chemical and aroma signals are generated simultaneously using a MD-GC-MS-O. Details on compounds in TIC are given in SI Table 9. Details on compounds in Aromagram are given in Table 5.

Table 5. Olfactometry results of residual VOC emitted from a plastic bag previously containing marijuana.

Event #	Descriptor	Hedonic Tone	Intensity	RT (min)	Width	Event Area
1	Solvent	Unpleasant -2	30	1.65	0.04	119
2	Medicinal, Aldehydic	Unpleasant -2	40	1.78	0.1	399
3	Ketone	Unpleasant -1	30	2.22	0.09	269
4	Sweet, Buttery	Pleasant +1	30	3.21	0.08	239
5	Solvent, Resiny	Unpleasant -1	30	4.00	0.14	419
6	Sweet	Pleasant +1	10	4.88	0.08	79
7	Grassy, Solvent	Neutral 0	60	5.99	0.3	1796
8	Medicinal, Resiny	Unpleasant -1	30	9.38	0.09	269
9	Potato, Moldy	Unpleasant -1	50	11.10	0.21	1048
10	Mint	Pleasant +1	20	11.55	0.07	139
11	Moldy, Mushroom, Potato	Unpleasant -1	40	13.45	0.19	758
12	Nutty, Mint	Pleasant +2	40	13.79	0.15	598
13	Burnt, Body odor	Unpleasant -2	50	14.17	0.17	848
14	Medicinal	Unpleasant -1	10	18.82	0.06	59
15	Resiny, Plastic	Unpleasant -1	30	19.86	0.16	479
16	Medicinal	Unpleasant -1	11	23.45	0.17	186
17	Woody, Mint	Neutral 0	30	25.88	0.24	718
18	Fruity	Pleasant +1	30	26.13	0.31	928

Event # corresponds to numbered peaks in Figure 10. “Characteristic” descriptor is used to represent the overall aroma of the sample (i.e. smell of marijuana). Hedonic tone is the overall pleasant or unpleasantness of the descriptor (range is Unpleasant -4, through 0, to Pleasant +4). Intensity is on a scale of 0-100, with 100 being most intense; intensity sets the peak height. RT = Retention Time. Width is defined as width at half-height of the Aromagram peak. Event area is a dimensionless value = Intensity x Width x 100, and is comparable to peak area counts generated with a mass selective detector.

2. Cocaine odor

1. Real cocaine odor vs. surrogate cocaine scent

Figure 11 compares concentration of volatiles emitted from 1 g of real cocaine and volatiles emitted from 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation. Aromatic compounds and phenols were not detected by MS in 1 g real cocaine samples. Acids, aromatics, halogenates, phenols, and sulfur containing volatiles were not detected by MS in 1 g surrogate cocaine scent. All compounds detected had published ODTs except hydrocarbons, ketones and nitrogen containing compounds. Finally, OAVs were not calculated for compounds that were not detected by MS (acids, aromatics, halogenates, phenols, and sulfur containing volatiles) or did not have ODTs (nitrogen containing). Current knowledge on odor impact is weakest regarding hydrocarbons, ketones, and nitrogen containing compounds in surrogate cocaine scent. Based on information presented, in order to make a more representative recipe that targets odor of 1 g cocaine, one would add or remove chemicals based on their calculated odor activity values to match the odor target (i.e., line up the solid line and dashed lines). For full details including identification, significant ions by MS, % spectral match by AMDIS, CAS, published odor descriptors, published ODTs, and calculated OAVs of the chemicals detected in headspace of all marijuana samples and surrogate scent marijuana formulation, please see SI Table 10, page 172.

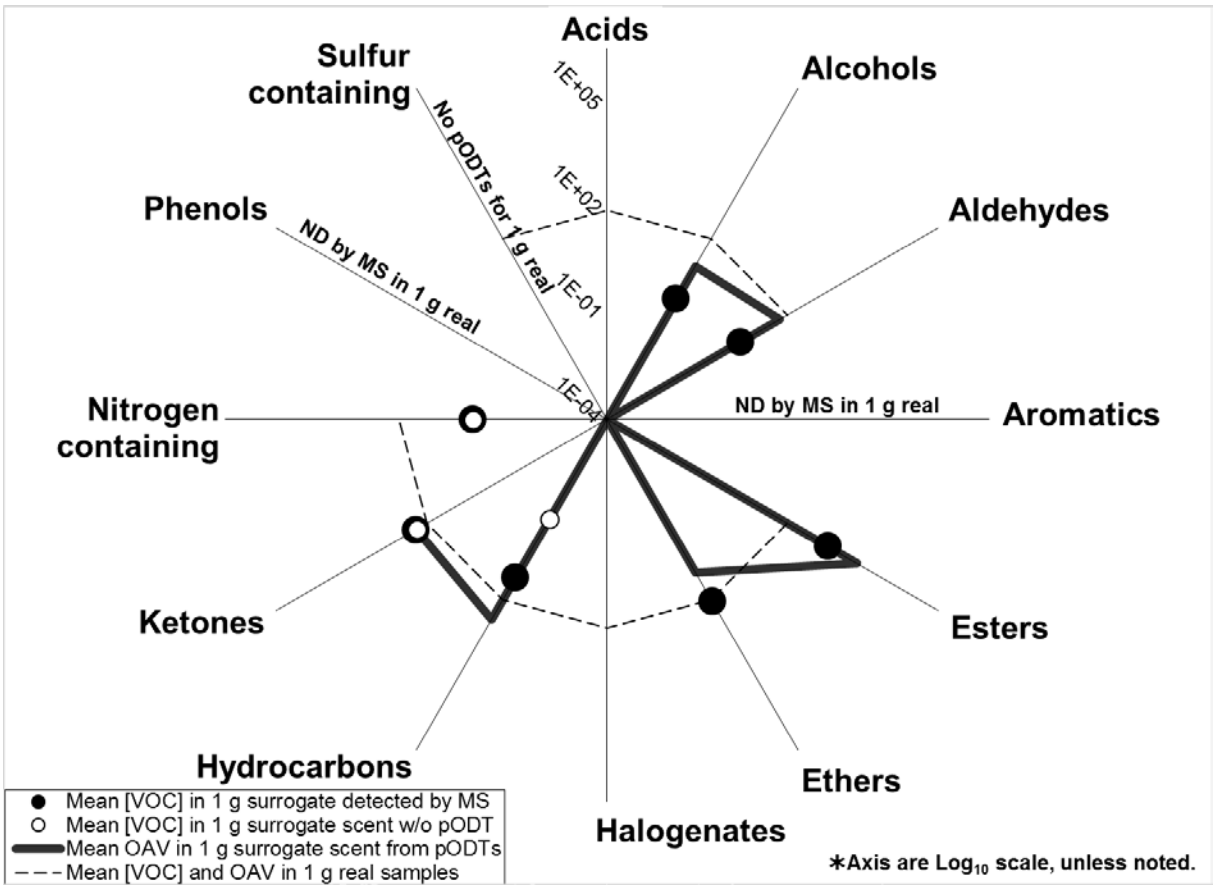

Figure 11. Comparison of VOC concentrations and odor activity values (OAVs) calculated from published odor detection values (ODTs) emitted from 1 g of real cocaine (represented as a reference dashed line at 100%) with 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation. The majority of chemical compound groups are mismatched with the target chemical content and odor impact, i.e., the position of solid black markers and solid line do not line up along the black dashed line, which would indicate 100% odor and chemical match on a % Log_{10} scale. Solid black markers indicate mean concentration of compounds detected by MS. White filled markers indicate the percentage of missing information in the form of no published ODTs available, i.e., the distance between these two markers indicates the level of current knowledge in odor impact of these compounds. An absent solid black line along a radial arm indicates compounds with no OAVs calculated (i.e. Acids, Aromatics, Halogenates, Nitrogen containing, Phenols, and Sulfur containing compounds), either because of no available published ODTs (i.e., Nitrogen and Sulfur containing) or were not detected, ND, (i.e., Acids, Aromatics, Halogenates, and Phenols). Aromatics and Phenols were not detected by MS in 1 g real cocaine (absent dashed line at 100%). Acids, Aromatics, Halogenates, Phenols, and Sulfur containing compounds were not detected by MS in 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation.

2. Effects of quantity of sample on cocaine odor perception

Odor profile was different between 1 g of cocaine and 1 kg of cocaine, i.e., generally, more sample mass lead to more volatiles emitted, in concentration and number of different compounds. Figure 12 illustrates the differences in concentration of volatiles emitted and associated odor impact of these volatiles between 1 g and 1 kg of cocaine. All chemical groups found in 1 kg real cocaine were found at or exceeding the concentration levels of 1 g real cocaine. Aromatics were found in 1 kg of cocaine and not found in 1 g cocaine samples, thus markers are shown in absolute value of MS detector response and not relative to 1 g real cocaine (100% dashed line). Sulfur containing volatiles were detected by MS in 1 g real cocaine, and not 1 kg real cocaine. These sulfur containing volatiles did not have published ODTs, thus no OAVs were calculated. Generally, with the exception of aromatics, where detection was in 1 kg cocaine and not in 1 g cocaine, the aroma profile between the two masses are similar. It is unknown whether the evidence bag had any interfering odors in the 1 kg sample; this possibility certainly needs to be taken into consideration for further odor analysis.

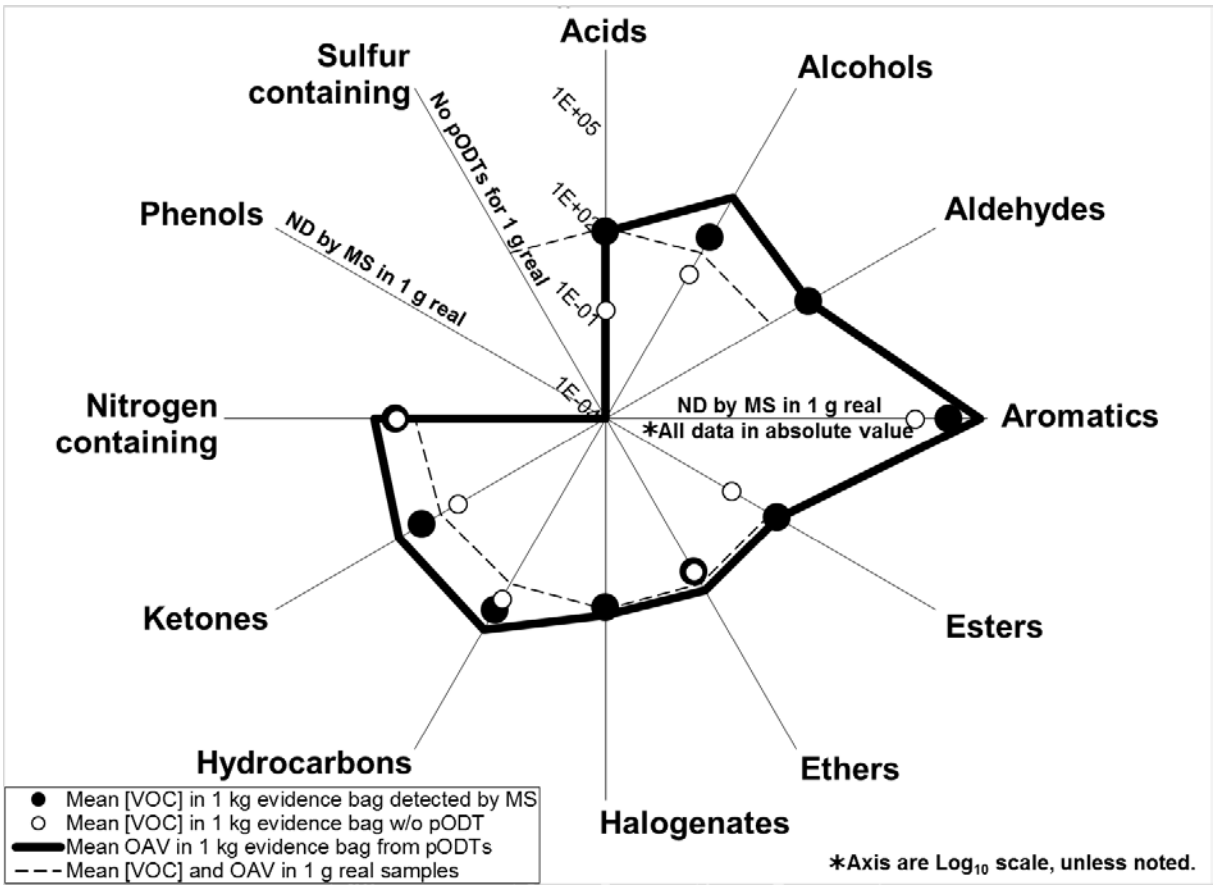

Figure 12. Comparison of VOC concentrations and odor activity values (OAVs) calculated from published odor detection values (ODTs) emitted from 1 g of real cocaine (represented as a reference dashed line at 100%) with 1 kg real cocaine in an evidence bag. The majority of chemical compound groups are matched with the target chemical content and odor impact, i.e., the position of solid black markers and solid line generally line up along the black dashed line, which would indicate 100% odor and chemical match on a % Log_{10} scale, with the exception of acids. Solid black markers indicate mean concentration of compounds detected by MS. White filled markers indicate the percentage of missing information in the form of no published ODTs available, i.e., the distance between these two markers indicates the level of current knowledge in odor impact of these compounds. An absent solid black line along a radial arm indicates compounds with no OAVs calculated (i.e. phenols and sulfur containing volatiles), because they were not detected, ND, (i.e., phenols and sulfur containing volatiles). Aromatics and Phenols were not detected by MS in 1 g real cocaine (absent dashed line at 100%).

3. Effects of adulterant on odor of cocaine

Figure 13 compares calculated OAVs based on published ODTs between 1 g real cocaine (light dashed line) and 1 g crack cocaine, 1 g cocaine with levamisole, and 1 g real surrogate cocaine scent. Rank of volatiles by odor impact, highest to lowest, for the odor of 1 g of real cocaine is acids, aldehydes, esters, ketones, alcohols, hydrocarbons, ethers, nitrogen containing, then halogenated volatiles. Rank of volatiles by odor impact, highest to lowest, for the odor of 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation scent is esters, ketones, aldehydes, alcohols, hydrocarbons, and then ethers. Rank of volatiles by odor impact, highest to lowest, for the odor of 1 g crack cocaine is acids, ketones, esters, aldehydes, aromatics, alcohols, nitrogen containing, ethers, and then hydrocarbons. Rank of volatiles by odor impact, highest to lowest, for the odor of 1 g cocaine with levamisole is aldehydes, ketones, alcohols, aromatics, hydrocarbons, nitrogen containing, and then acids. Figure 13 illustrates how 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation is not a representative odor mimic for the types of illicit cocaine sampled in Table 3, i.e., the solid black line is not congruent with any of the other lines. More importantly, since none of the lines are congruent, this information suggests that 1 single surrogate scent formulation would not be appropriate to use as a training tool to mimic the odor of cocaine in various packaging, various masses, various forms (i.e., freebase, cut with levamisole) found in forensic applications.

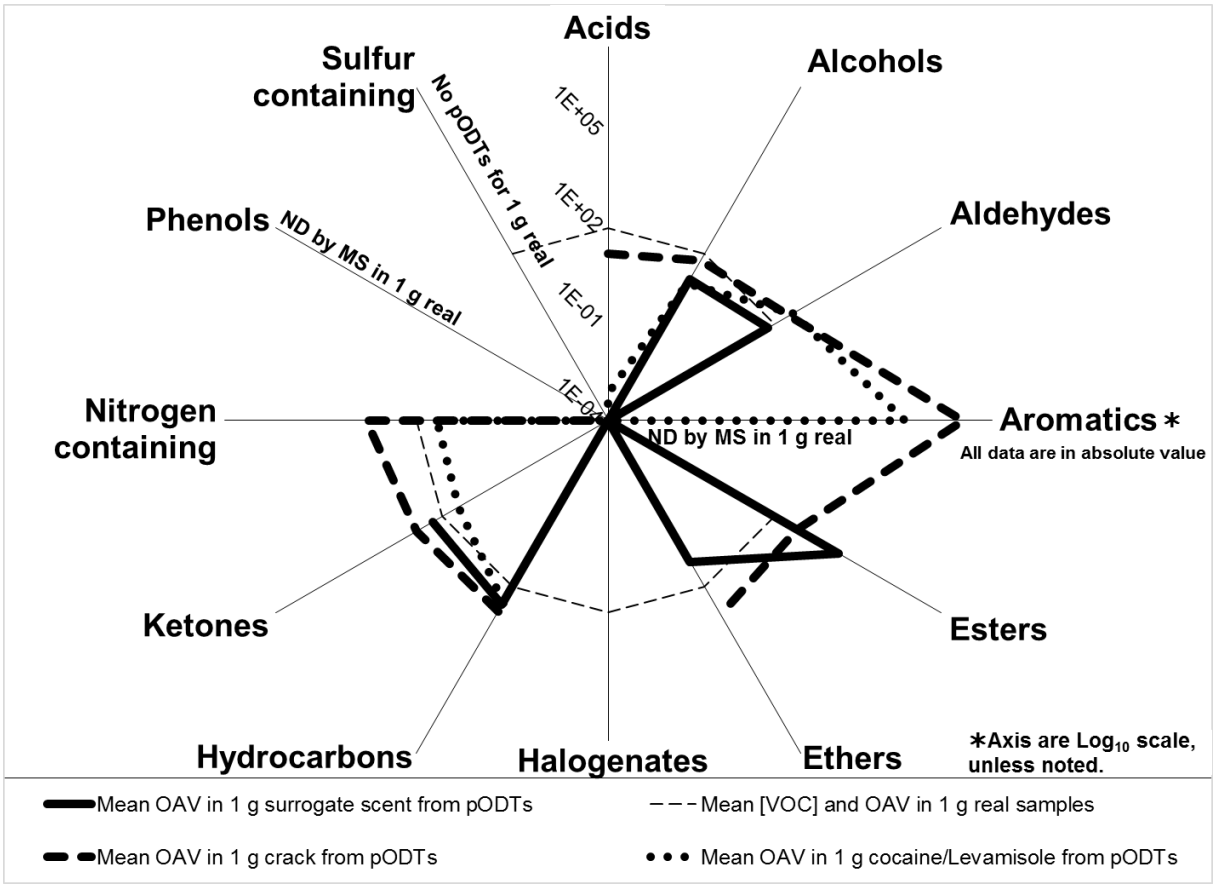

Figure 13. Cocaine odor is not a one-size-fits-all recipe for all states of seizure. A comparison of calculated odor activity values (OAVs) with published odor detection values (ODTs) emitted from 1 g of real cocaine (represented as a reference dashed line at 100%) with 1 g crack cocaine, 1 g cocaine cut with levamisole, and 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation is shown. The majority of chemical compound groups are mismatched with the odor impact, i.e., the position of all the lines do not match up, which would indicate 100% odor match on a % Log_{10} scale. Sigma Pseudo™ Narcotic Scent Cocaine formulation is not a comprehensive odor mimic for the types of cocaine samples analyzed in this study.

4. Simultaneous chemical and sensory analysis of cocaine

Figure 14 is an aromagram depicting the odor of 1 g real cocaine and 1 g Sigma Pseudo™ Narcotic Scent Cocaine as detected by human nose. There were 7 aroma events detected in 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation and 27 aroma events in 1 g real cocaine. The descriptor “characteristic” is used to describe the

aroma that represents the overall scent of cocaine, here reported at retention times 19.13 and 19.89 min. Full details on odor description, hedonic tone, intensity, and retention time for each peak are given in Table 6 and Table 7.

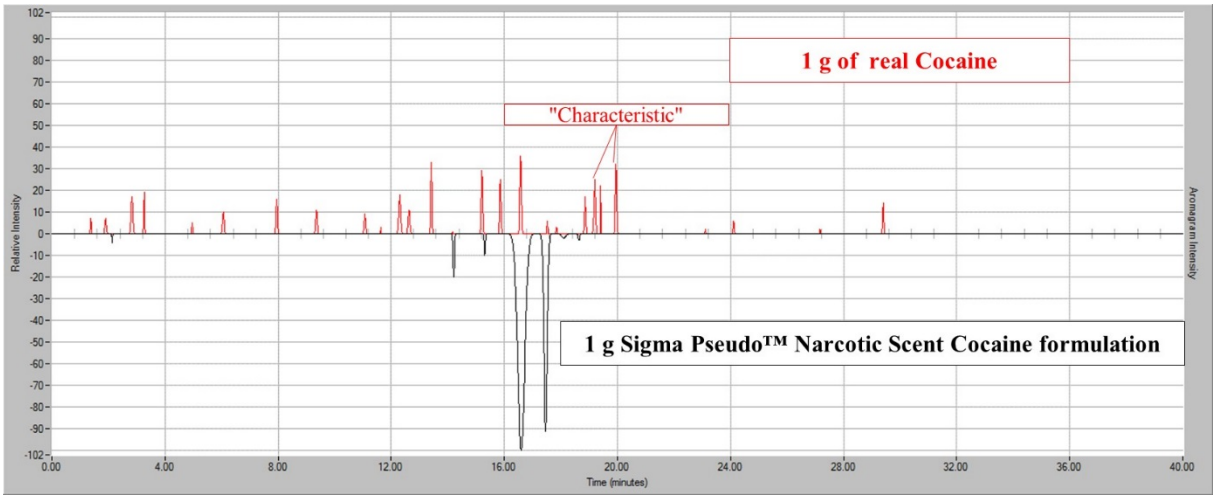

Figure 14. Example of aromagrams of 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation vs. 1 g of real cocaine. Overlay of aromagrams generated with olfactometry data of Sigma Pseudo™ Narcotic Scent Cocaine formulation (inverted black signal, "E1" from Table 3, aroma details in Table 6) and 1 g illicit cocaine, in an opened bag (red signal, D5 of Table 3, details in Table 7). “Characteristic” descriptor is used to tag an odor component that represents the overall aroma of the sample (i.e. smell of cocaine).

Figure 15 is an example of a typical overlay of TIC with aromagram, depicting the simultaneous chemical (red signal) and sensory analysis (black signal) of 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation, respectively. For the lot of Sigma Pseudo™ Narcotic Scent Cocaine formulation analyzed in this study, the ingredients are listed as pyrogenic colloidal silica (1%), cellulose (98.9%), methyl benzoate (0.1%). Of these 3 ingredients, methyl benzoate was detected (CAS 93-58-3, retention time 16.30 min, See SI Table 10), and described by human panelist as “sweet, unknown”. Previously published odor characteristics of methyl benzoate are reported as “prune,

lettuce, herb, sweet” and “phenolic”. There were no aroma events flagged in the 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation as a characteristic odor of cocaine. This analysis highlights how there might be more odors present than intended in Sigma Pseudo™ Narcotic Scent Cocaine formulation, leading to misidentification by odor in the case of drug detection canines. Full details of odor character, hedonic tone, and intensity are given in Table 6.

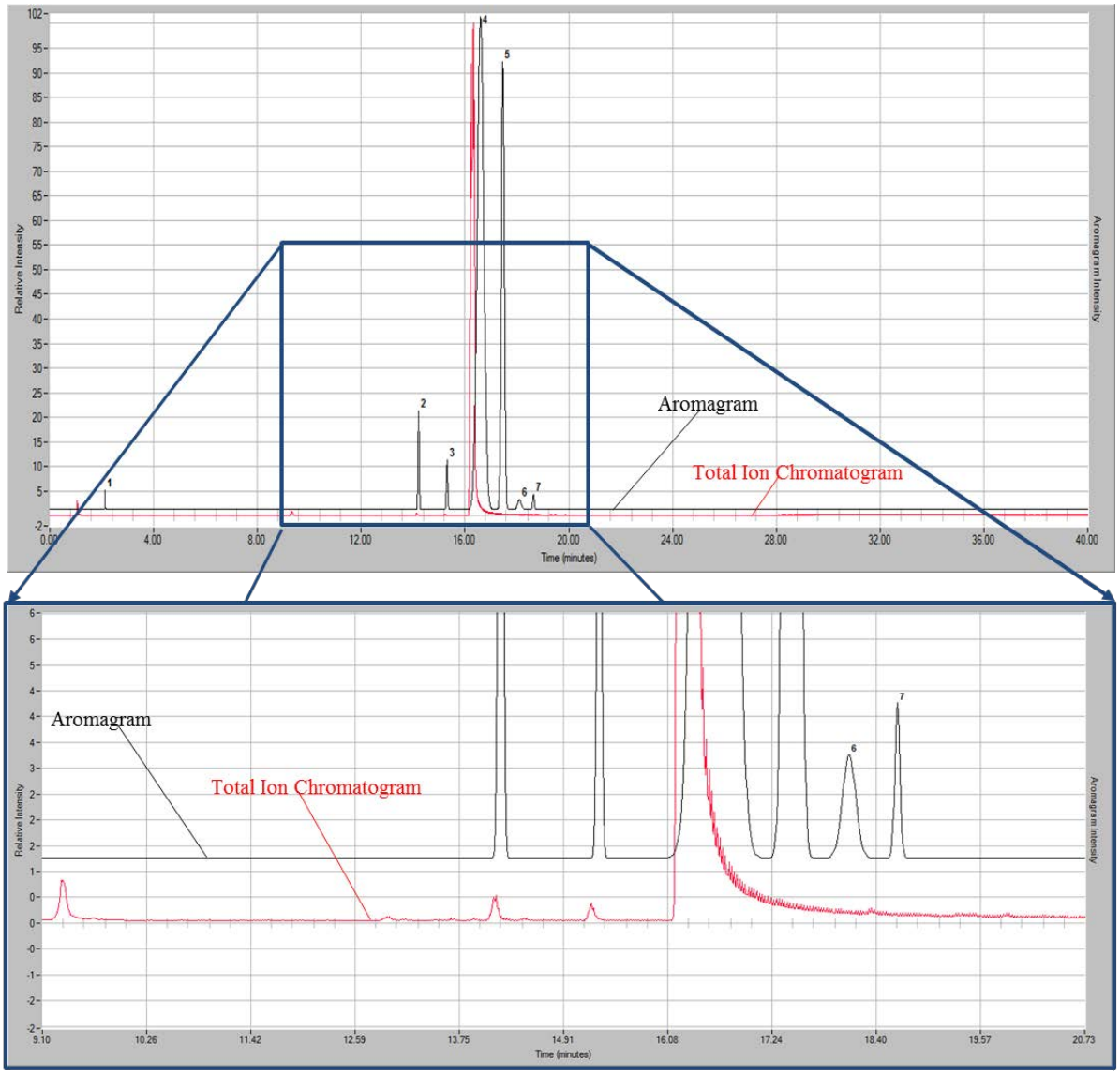

Figure 15. Example of a typical overlay of total ion chromatogram and aromagram of 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation. 1 h, static, extraction at room temperature of 1 g of Sigma Pseudo™ Narcotic Scent Cocaine formulation using Carboxen/PDMS SPME fiber. Chemical and aroma signals are generated simultaneously using a MD-GC-MS-O. Details on compounds in TIC are given in SI Table 10. Details on compounds in aromagram are given in Table 6. Zoomed view shows mis/match of aromas detected and chemicals detected.

Table 6. Olfactometry results of sensory analysis of 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation using MD-GC-MS-O

Event #	Descriptor	Hedonic Tone	Intensity	RT (min)	Width	Event Area
1	Unknown	Unpleasant -1	4	2.11	0.05	19
2	Buttery	Pleasant +2	20	14.15	0.13	259
3	Unknown	Unpleasant -4	10	15.25	0.49	129
4	Sweet, Unknown	Unpleasant -4	100	16.36	0.69	6888
5	Unknown	Neutral 0	91	17.31	0.31	2816
6	Unknown	Neutral 0	2	17.9	0.41	81
7	Grassy	Neutral 0	3	18.57	0.16	47

Event # corresponds to numbered peaks Figure 15. "Characteristic" descriptor is used to represent the overall aroma of the sample (i.e. smell of cocaine). Hedonic tone is the overall pleasant or unpleasantness of the descriptor (range is Unpleasant -4, through 0, to Pleasant +4). Intensity is on a scale of 0-100, with 100 being most intense; intensity sets the peak height. RT = Retention Time. Width is defined as width at half-height of the Aromagram peak. Event area is a dimensionless value = Intensity x Width x 100, and is comparable to peak area counts generated with a mass selective detector.

Similar analysis of 1 g real cocaine odor showed similar results. There are intense odors present when simultaneous chemical analysis by MS show only background signal. The most abundant chemical peak at 12.10 minutes was identified as acetic acid, with panelist tagged descriptor and published odor character reported as "acidic" and "sour". This compound was not found in 1 g Sigma Pseudo™ Narcotic Scent Cocaine formulation, but found in 1 g of real cocaine, and cocaine in an evidence bag. It is unclear whether acetic acid is an artifact of plastic packaging, no true blank plastic packaging was available for comparison. The most intense odor (event # 17) has very small simultaneous chemical signal, with possible identification as acetophenone, 3-ethyltoluene, or 2, 2, 4-trimethylpentane (retention times 16.49-16.53

min, **SI Table** 10) by AMDIS. Complete odor identification given in Table 7. This analysis is a great example of how a big chemical peak does not equate to big odor impact when using the concept of odor activity values. Most of the odorous compounds emitted from 1 g cocaine samples could have low odor detection thresholds, allowing for detection by smell and not by MS.

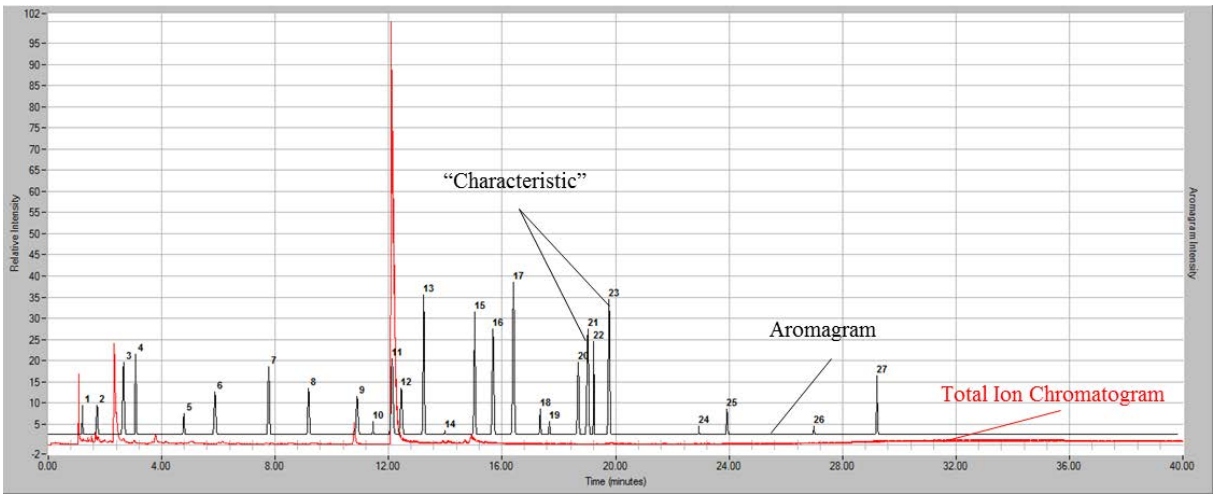

Figure 16. Example of typical overlay of total ion chromatogram and aromagram of illicit cocaine (opened bag) using MD-GC-MS-O (D5, see Table 3). 1 h, static, room temperature extraction of VOCs emitted into headspace from 1 g of illicit cocaine, in an opened plastic bag, using Carboxen/PDMS SPME fiber. Chemical and aroma signals are generated simultaneously using a MD-GC-MS-O. Details on compounds in TIC are given in SI Table 10. Details on compounds in Aromagram are given in Table 7.

Table 7. Olfactometry results of VOCs emitted from illicit cocaine using MD-GC-MS-O.

Event #	Descriptor	Hedonic Tone	Intensity	RT (min)	Width	Event Area
1	Unknown	Neutral 0	7	1.35	0.08	55
2	Chocolate	Pleasant +2	7	1.84	0.14	97
3	Chocolate, Earthy	Pleasant +1	17	2.76	0.16	271
4	Buttery	Pleasant +1	19	3.22	0.09	170
5	Sweet	Pleasant +1	5	4.92	0.09	44
6	Grassy	Neutral 0	10	5.99	0.15	149
7	Pine	Unpleasant -1	16	7.89	0.13	207
8	Unknown	Neutral 0	11	9.29	0.14	153
9	Mint	Pleasant +1	9	10.99	0.16	143
10	Unknown	Neutral 0	3	11.61	0.04	11
11	Acidic	Unpleasant -4	18	12.11	0.19	341
12	Sweet, Floral	Pleasant +2	11	12.55	0.18	197
13	Unknown	Neutral 0	33	13.37	0.11	362
14	Unknown	Neutral 0	1	14.15	0.05	4
15	Unknown	Pleasant +3	29	15.15	0.13	376
16	Dirt	Neutral 0	25	15.79	0.14	349
17	Sweat, Body odor	Unpleasant -3	36	16.51	0.14	503
18	Milky	Neutral 0	6	17.48	0.08	47
19	Musk	Pleasant +2	3	17.81	0.09	26
20	Unknown	Neutral 0	17	18.8	0.14	237
21	**Characteristic**	Neutral 0	25	19.13	0.16	399
22	Woody	Pleasant +1	22	19.39	0.06	131
23	**Characteristic**	Neutral 0	32	19.89	0.13	415
24	Unknown	Neutral 0	2	23.09	0.06	11
25	Unknown	Pleasant +1	6	24.07	0.1	59
26	Burnt leaves	Unpleasant -2	2	27.12	0.1	19
27	Woody, Plant	Unpleasant -1	14	29.35	0.1	139

Event # corresponds to numbered peaks in Figure 16. “Characteristic” descriptor is used to represent the overall aroma of the sample (i.e. smell of cocaine). Hedonic tone is the overall pleasant or unpleasantness of the descriptor (range is Unpleasant -4, through 0, to Pleasant +4). Intensity is on a scale of 0-100, with 100 being most intense; intensity sets the peak height. RT = Retention Time. Width is defined as width at half-height of the Aromagram peak. Event area is a dimensionless value = Intensity x Width x 100, and is comparable to peak area counts generated with a mass selective detector.

3. Heroin odor

A. Effects of age of the drug

Two samples of heroin were analyzed, one seized in 1997 and the other seized in 2010, places of origin are unknown. 1 g of 2010 heroin is used to calculate 100% concentration and odor impact line of Figure 17. The increase in acids by 2 orders of magnitude is almost entirely due to acetic acid (retention time 12.09 min, SI Table 11). Increased age of heroin shows an increase in the following volatiles detected by MS: aromatics, ethers, and halogenates. Increased age of heroin also shows an increase in odor impact of acids, alcohols, aromatics, esters, ketones and nitrogen containing volatile compounds. The most odorous chemical groups in heroin seized in 2010, ordered most to least, is aldehydes, acids, ethers, hydrocarbons, esters, alcohols, ketones, aromatics, and then nitrogen containing volatiles. The most odorous chemical groups in heroin seized in 1997, ordered most to least, is acids, aldehydes, aromatics, alcohols, hydrocarbons, ethers, ketones, nitrogen containing and then esters. The most odorous chemical groups in 1 g of Sigma Pseudo™ Narcotic Scent Heroin formulation, ordered most to least, is acids, aromatics, ketones, esters, aldehydes, alcohols, ethers, hydrocarbons, and then nitrogen containing volatiles. Halogenates were found only in 1997 heroin, but no published ODTs were found, thus no OAVs were calculated. Phenols and sulfur containing volatiles were not detected by MS in any of the 3 heroin samples. It would appear, at least visually, that 1 g of Sigma Pseudo™ Narcotic Scent Heroin formulation is a closer odor mimic to heroin from 1997, and not a more recently seized sample, but it is noted that origin and subsequent treatment of 1997 and 2010 heroin is unknown.

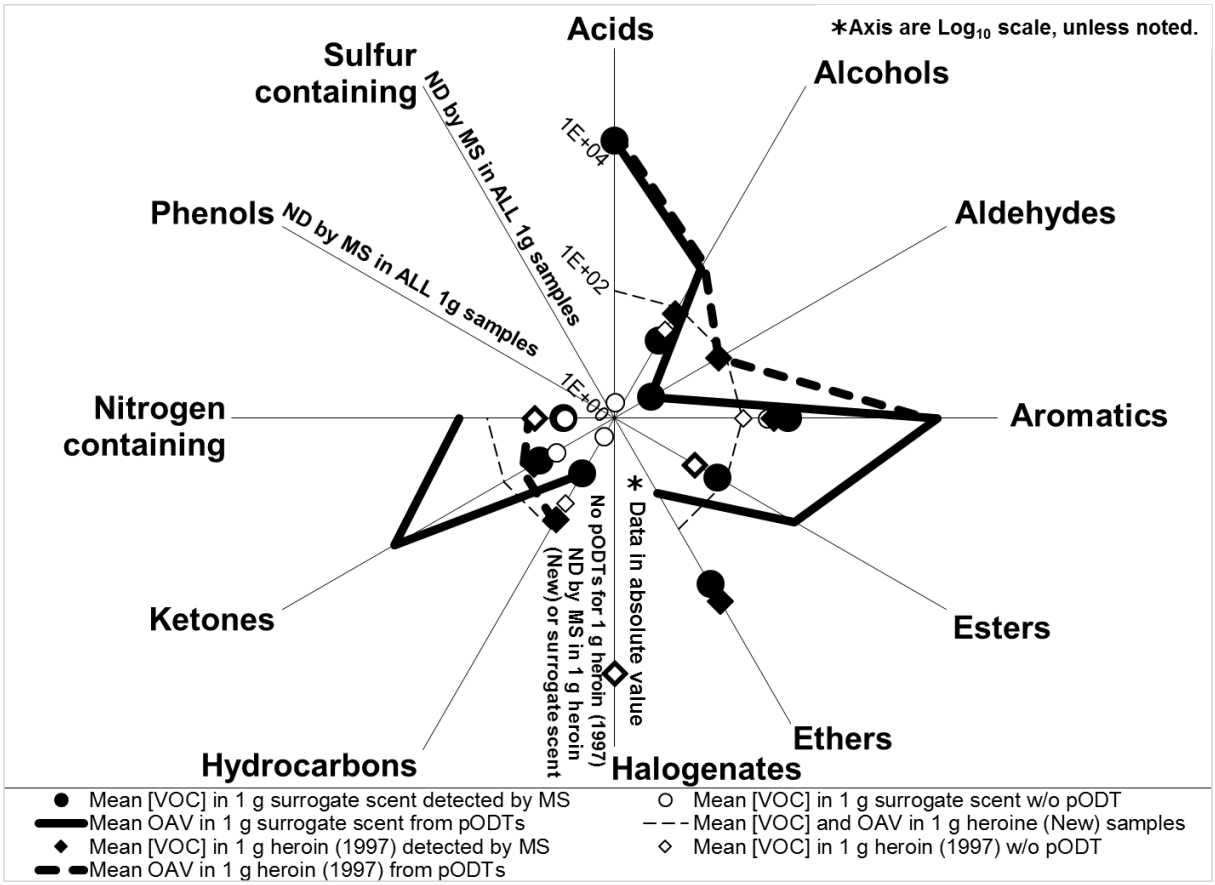

Figure 17. Heroin odor is not a one-size-fits-all recipe for all states of seizure. A comparison of calculated odor activity values (OAVs) with published odor detection values (ODTs) emitted from 1 g of heroin from 2010 (represented as a reference dashed line at 100%) with 1 g heroin from 1997, and 1 g Sigma Pseudo™ Narcotic Scent Heroin formulation is shown. The majority of chemical compound groups are mismatched with the odor impact, i.e., the position of all the OAV lines do not match up, which would indicate 100% odor match on a % Log_{10} scale. Sigma Pseudo™ Narcotic Scent Heroin formulation is not a comprehensive odor mimic for the types of heroin samples analyzed in this study.

B. Simultaneous chemical and sensory analysis of heroin

Figure 18 is an example of a typical overlay of TIC with aromagram, depicting the simultaneous chemical (red signal) and sensory analysis (black signal) of 1 g Sigma Pseudo™ Narcotic Scent Heroin formulation, respectively. The MSDS of Sigma Pseudo™ Narcotic Scent Marijuana formulation analyzed in this study, lists the ingredients as pyrogenic colloidal silica (0.3%), cellulose (74.1%), o-acetylsalicylic acid (25.2%), and acetic acid (0.3%). Of these 4 ingredients, acetic acid (CAS 64-19-7, retention time 12.09 min, See **SI Table** 11) was detected by the method, and described by human panelist as “acidic”. Previously published odor characteristics of acetic acid are reported as “sour” and “acidic. There was no human olfactometry analysis of real heroin, thus only the TIC and aromagram of Sigma Pseudo™ Narcotic Scent Heroin formulation are presented. This analysis, with full chemical analysis in **SI Table** 11, highlights how there are more possible odors in real heroin, shown in OAVs, than the smell of vinegar. Training to a couple of odors in surrogate heroin scent can lead to misidentification by odor in the case of drug detection canines. Full details of odor character, hedonic tone, and intensity are given in Table 8.

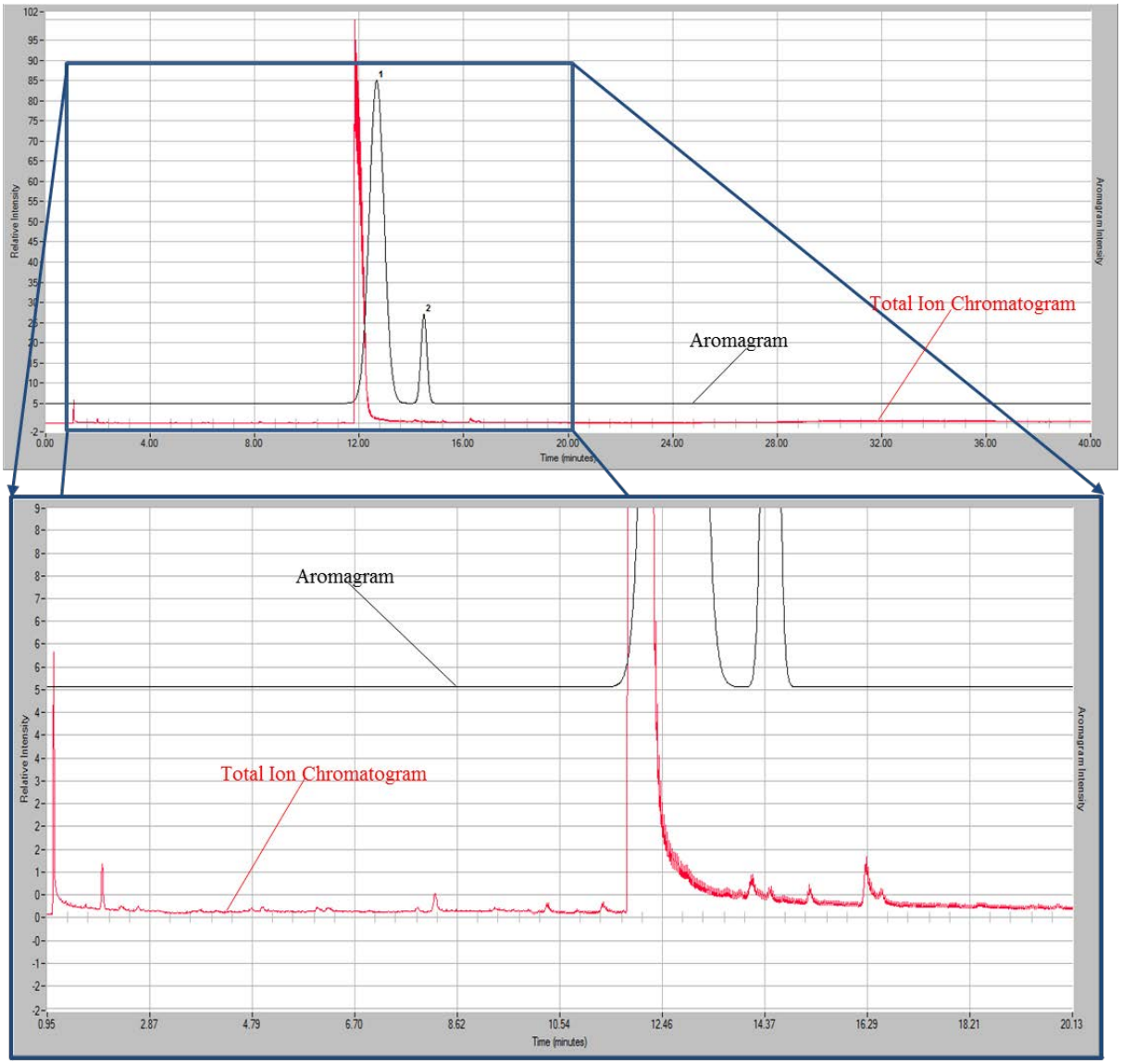

Figure 18. Example of a typical overlay of total ion chromatogram and aromagram of Heroin Pseudo Scent. 1 h, static, extraction at room temperature of 1 g of Sigma Pseudo Scent Heroin using Carboxen/PDMS SPME fiber. Chemical and aroma signals are generated simultaneously using a MD-GC-MS-O. Details on compounds in TIC are given in SI Table 11. Details on compounds in aromagram are given in Table 8. Zoomed view show mis/match of aromas detected and chemicals detected.

Table 8. Olfactometry results of sensory analysis of Heroin Pseudo Scent

Event #	Descriptor	Hedonic Tone	Intensity	RT (min)	Width	Event Area
1	Acidic	Unpleasant -3	80	12.10	1.56	12459
2	Buttery, Rusty, Sweet	Unpleasant -1	22	14.18	0.62	1361

Event# corresponds to numbered peaks in Figure 18. Hedonic tone is the overall pleasant or unpleasantness of the descriptor (range is Unpleasant -4, through 0, to Pleasant +4). Intensity is on a scale of 0-100, with 100 being most intense; intensity sets the peak height. RT = Retention Time. Width is defined as width at half-height of the Aromagram peak. Event area is a dimensionless value = Intensity x Width x 100, and is comparable to peak area counts generated with a mass selective detector.

Conclusions

The data presented in this study show that there is not a direct linear relationship between chemical concentration (i.e., abundance of the compound in headspace) and odor impact (i.e., calculated odor activity values from published odor detection thresholds). It is shown that odor impact is influenced more by the odor detection threshold of a compound.

This reports seeks to point out the gaps in the evaluation of odor of marijuana, cocaine, and heroin. There are highly odorous compounds present in headspace of these drugs, with very low odor detection thresholds, that are likely mainly responsible for the overall odor of these drugs. Previous reports of the most abundant compounds in headspace can mislead researchers when dealing with odor of these compounds. Surrogate scent formulations, therefore, need to mimic the odor impact of key compounds and not just the chemical abundance of compounds detected. When manufacturing these standards, utmost care needs to be taken to ensure contaminating

odors are not added. It is shown that if the ODT is very small, even very small amounts of the contaminant contribute to the overall odor of the surrogate training tool.

The use of SPME allowed VOCs in headspace to be extracted and pre-concentrated on site, and analyzed by MDGC-MS-O. This state of the art instrumentation allowed for further separation of odorous compounds and simultaneous detection by human nose to further elucidate the separate odor parts that make up the whole of the total aroma of these drugs. The concept of odor activity value, then, is useful to researchers without such instrumentation. OAVs can be calculated from published ODTs. More research is warranted to expand the database, and determine ODTs for compounds of interest.

References

1 Schnabel, K. O., Belitz, H. D. & Vonranson, C. Investigations on the structure-activity-relationsthips of odorous substances 1. Detection thresholds and odor qualities of alophatic and alicyclic compounds containing oxygen functions. *Zeitschrift Fur Lebensmittel-Untersuchung Und-Forschung* **187**, 215-223, doi:10.1007/bf01043342 (1988).

2 Yoshii, F., Yamada, Y., Hoshi, T. & Hagiwara, H. The creation of a database of odorous compounds focused on molecular rigidity and analysis of the molecular features of the compounds in the database. *Chemical Senses* **27**, 399-405, doi:10.1093/chemse/27.5.399 (2002).

3 Yoshii, F. & Hirono, S. Construction of a quantitative three-dimensional model for odor quality using comparative molecular field analysis (CoMFA). *Chemical Senses* **21**, 201-210, doi:10.1093/chemse/21.2.201 (1996).

4 Cometto-Muniz, J. E., Cain, W. S., Abraham, M. H. & Gil-Lostes, J. Concentration-detection functions for the odor of homologous n-acetate esters. *Physiology & Behavior* **95**, 658-667, doi:10.1016/j.physbeh.2008.09.021 (2008).

5 Leonardos, G., Kendall, D., Barnard, N. & Little, A. D., Inc. Odor threshold determinations of 53 odorant chemicals. *Journal of Air Pollution Control Association* **19**, 91-95, doi:10.1080/00022470.1969.10466465 (1969).

6 Patton, S. & Josephson, D. V. A method for determining significance of volatile flavor compounds in foods. *Food Res* **22**, 316-318 (1957).

7 Clery, R. High-impact odorants in essential oils. *Flavour and Fragrance Journal* **25**, 117-120, doi:10.1002/ffj.1980 (2010).

8 Sacks, G. L. *et al.* Sensory Threshold of 1,1,6-Trimethyl-1,2-dihydronaphthalene (TDN) and Concentrations in Young Riesling and Non-Riesling Wines. *Journal of Agricultural and Food Chemistry* **60**, 2998-3004, doi:10.1021/jf205203b (2012).

9 Parker, D. B. *et al.* Odor and odorous chemical emissions from animal buildings: Part 6. odor activity value. *Transactions of the Asabe* **55**, 2357-2368 (2012).

10 Cometto-Muniz, J. E. & Abraham, M. H. Odor Detection by Humans of Lineal Aliphatic Aldehydes and Helional as Gauged by Dose-Response Functions. *Chemical Senses* **35**, 289-299, doi:10.1093/chemse/bjq018 (2010).

11 Kim, K.-H. & Park, S.-Y. A comparative analysis of malodor samples between direct (olfactometry) and indirect (instrumental) methods. *Atmospheric Environment* **42**, 5061-5070, doi:10.1016/j.atmosenv.2008.02.017 (2008).

12 Cai, L., Koziel, J. A. & O'Neal, M. E. Determination of characteristic odorants from Harmonia axyridis beetles using in vivo solid-phase microextraction and multidimensional gas chromatography-mass spectrometry-olfactometry. *Journal of Chromatography A* **1147**, 66-78, doi:10.1016/j.chroma.2007.02.044 (2007).

13 Dekeirsschieter, J. *et al.* Cadaveric volatile organic compounds released by decaying pig carcasses (Sus domesticus L.) in different biotopes. *Forensic Science International* **189**, 46-53, doi:10.1016/j.forsciint.2009.03.034 (2009).

14 Alexander, M. B., Hodges, T. K., Bytheway, J. & Aitkenhead-Peterson, J. A. Application of soil in Forensic Science: Residual odor and HRD dogs. *Forensic Science International* **249**, 304-313, doi:10.1016/j.forsciint.2015.01.025 (2015).

15 Harvey, L. M. & Harvey, J. W. Reliability of bloodhounds in criminal investigations. *Journal of Forensic Sciences* **48**, 811-816 (2003).

16 Vyplelova, P. *et al.* Individual human odor fallout as detected by trained canines. *Forensic Science International* **234**, 13-15, doi:10.1016/j.forsciint.2013.10.018 (2014).

17 Voss, A. *et al.* Detecting Cannabis Use on the Human Skin Surface via an Electronic Nose System. *Sensors* **14**, 13256-13272, doi:10.3390/s140713256 (2014).

18 Tipple, C. A. *et al.* Comprehensive characterization of commercially available canine training aids. *Forensic Science International* **242**, 242-254, doi:10.1016/j.forsciint.2014.06.033 (2014).

19 Kranz, W. *et al.* On the smell of Composition C-4. *Forensic Science International* **236**, 157-163, doi:10.1016/j.forsciint.2013.12.012 (2014).

20 Lorenzo, N. *et al.* Laboratory and field experiments used to identify Canis lupus var. familiaris active odor signature chemicals from drugs, explosives, and humans. *Analytical and Bioanalytical Chemistry* **376**, 1212-1224, doi:10.1007/s00216-003-2018-7 (2003).

21 Macias, M. S., Harper, R. J. & Furton, K. G. A comparison of real versus simulated contraband VOCs for reliable detector dog training utilizing SPME-GC-MS. *American Laboratory* **40**, 16-+ (2008).

22 Chen, S., Xu, Y. & Qian, M. C. Aroma Characterization of Chinese Rice Wine by Gas Chromatography-Olfactometry, Chemical Quantitative Analysis, and Aroma Reconstitution. *Journal of Agricultural and Food Chemistry* **61**, 11295-11302, doi:10.1021/jf4030536 (2013).

23 Ohloff, G. in *Perfumer & Flavorist* Vol. 3 11-22 (1978).

24 M. Devos, F. P., J. Rouault, P. Laffort, L.J. Van Gemert. *Standardized Human Olfactory Thresholds*. (IRL Press at Oxford Press, 1990).

25 Rice, S. & Koziel, J. A. *Characterizing the smell of marijuana by odor impact of volatile compounds. An application of simultaneous chemical and sensory analysis.* (2015).

CHAPTER 5. THE RELATIONSHIP BETWEEN CHEMICAL CONCENTRATION AND ODOR ACTIVITY VALUE EXPLAINS THE INCONSISTENCY IN MAKING A COMPRENSIVE SURROGATE SCENT TRAINING TOOL REPRESENTATIVE OF ILLICIT DRUGS (SUPPORTING INFORMATION)

Modified from a paper submitted to *Forensic Science International*

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SI Table 9. Summary of VOCs emitted from all real marijuana samples and Sigma Pseudo™ Scent Marijuana formulation over 1 hour at room temperature. Sigma Pseudo™ Scent Marijuana formulation is indicated by <u>underlined</u> and **bolded** fonts..

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
Ethylene oxide	**75-21-8**	**1.07**				**8.51E+02**	A 1	2: 44 45	66	1.51E+06	1.77E+03
							A 3		66	2.12E+06	2.49E+03
							A 4		65	3.37E+06	3.96E+03
							A 7	2: 43 42	89	8.62E+03	1.01E+01
							B 1	2: 44 43	66	3.75E+06	4.40E+03
							B 4	4: 44 45 129 43	66	1.86E+06	2.18E+03
							<u>C 1</u>	<u>3: 44 45 46</u>	<u>66</u>	<u>1.35E+06</u>	<u>1.59E+03</u>
							<u>C 2</u>	<u>2: 44 43</u>	<u>85</u>	<u>2.14E+05</u>	<u>2.51E+02</u>
							<u>C 3</u>	<u>4: 44 46 43 131</u>	<u>67</u>	<u>1.36E+06</u>	<u>1.60E+03</u>
2-nitropropane	79-46-9	1.13				7.24E+00	A 5	2: 41 43	75	6.30E+03	8.69E+02
							A 6	4: 43 39 56 42	83	4.16E+04	5.74E+03
2,4-dimethylpentane	108-08-7	1.20				8.71E+01	A 7	2: 57 43	66	8.15E+03	9.36E+01
Isobutane	75-28-5	1.22				1.00E+01	A 1		84	2.20E+07	2.20E+06
							A 2	13: 43 41 57 72 39 55 56 38 40 73 62 66 65	84	2.02E+07	2.02E+06
							A 3	11: 43 42 41 57 72 40 53 51 38 73 63	85	1.47E+07	1.47E+06
							A 4	5: 57 42 43 41 39	67	2.03E+04	2.03E+03
							A 5	10: 43 42 41 39 72 55 50 73 71 58	84	7.18E+06	7.18E+05
							A 6	4: 43 39 56 42	88	4.16E+04	4.16E+03
							A 7	10: 43 42 41 57 39 72 55 56 73 37	85	2.94E+06	2.94E+05
							B 1	14: 43 42 41 57 72 39 56 55 71 50 70 53 38 37	85	2.20E+06	2.20E+05
							B 2	7: 42 41 72 53 55 56 38	84	7.00E+05	7.00E+04

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 3	4: 43 42 41 39	88	2.49E+04	2.49E+03
							B 4	4: 42 43 57 72	81	6.45E+04	6.45E+03
Acetaldehyde	**75-07-0**	**1.27**	**Pungent, Ether**	**Pungent, Ethereal, Aldehydic, Fruity**	**1.50E-02**	**1.86E-01**	A 4	2: 44 42	91	3.10E+04	1.67E+05
							A 6	2: 43 44	90	2.69E+04	1.44E+05
							A 7	2: 43 42	88	8.62E+03	4.63E+04
							B 2		89	6.11E+03	3.28E+04
							B 3		96	2.85E+04	1.53E+05
							B 4	2: 44 43	96	8.88E+04	4.77E+05
							C 2	2: 43 44	95	2.95E+04	1.58E+05
							C 3	2: 43 41	96	6.95E+04	3.73E+05
Trichloromonofluoromethane	75-69-4	1.27					B 1	2: 103 101	75	4.34E+03	
							B 4	2: 101 103	81	1.72E+04	
2,3-dimethylbutane	79-29-8	1.28					A 6	3: 43 71 42	73	1.06E+04	
							B 2		66	5.01E+03	
							B 3	4: 43 42 41 39	71	2.49E+04	
Ethylenimine	151-56-4	1.30					A 5	1: 41	70	5.22E+04	
							A 6	3: 43 42 39	81	2.30E+04	
							B 2		81	5.01E+03	
							B 3	4: 43 42 41 39	83	2.49E+04	
Ethyl ether	60-29-7	1.31		Ethereal			B 2	1: 59	86	2.37E+04	
Ketene	**463-51-4**	**1.31**					A 4		80	3.54E+03	
							A 7	3: 41 42 59	74	3.81E+04	
							B 1	3: 42 41 55	72	1.04E+05	
							C 2	2: 41 42	73	3.11E+03	
Isoprene	**78-79-5**	**1.33**					A 4	3: 39 53 51	85	3.34E+04	
							A 5	1: 67	71	1.73E+04	
							A 7		93	3.12E+04	
							B 1	3: 67 53 65	69	2.08E+04	
							B 3		77	4.59E+03	
							B 4	5: 67 51 41 53 66	95	7.61E+04	
							C 3	3: 67 39 53	81	1.42E+04	
(E)-1,3-Pentadiene	2004-70-8	1.34					B 4		94	2.13E+04	
1,3-Pentadiene	504-60-9	1.34					B 4		94	2.13E+04	
Hexane	110-54-3	1.34	Alkane			2.19E+01	A 1	7: 41 76 57 56 86 43 39	69	1.33E+05	6.09E+03
							A 2	4: 62 56 42 86	66	2.53E+04	1.16E+03
							A 3	2: 56 41	88	8.55E+04	3.91E+03
							A 4	5: 57 42 43 41 39	78	2.03E+04	9.27E+02
							A 5	2: 41 57	75	1.84E+04	8.43E+02

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 6	4: 76 42 56 43	74	1.57E+05	7.18E+03
							A 7	1: 86	86	5.53E+04	2.53E+03
							B 1	2: 57 56	79	3.71E+04	1.69E+03
							B 2	2: 43 57	74	3.37E+04	1.54E+03
							B 3		67	2.96E+04	1.35E+03
							B 4		81	1.82E+04	8.32E+02
4-methyldecane	2847-72-5	1.39					A 1	12: 43 42 71 41 57 39 70 55 56 86 38 69	66	2.55E+06	
							A 2	13: 43 71 42 41 57 70 39 56 86 85 62 54 63	66	2.66E+06	
							A 3	17: 43 42 41 70 86 56 50 40 57 38 65 63 51 69 37 85 67	65	4.43E+06	
							A 4		75	1.66E+04	
							A 5	10: 39 57 55 41 86 53 69 38 52 67	66	1.35E+06	
							A 7		65	6.20E+05	
							B 1	10: 43 42 41 56 57 39 85 86 69 54	65	8.52E+05	
2-methylpentane	107-83-5	1.39					A 1	12: 43 42 71 41 57 39 70 55 56 86 38 69	98	2.55E+06	
							A 2	13: 43 71 42 41 57 70 39 56 86 85 62 54 63	98	2.66E+06	
							A 3	3: 67 87 85	98	4.89E+06	
							A 4	2: 43 41	80	1.89E+04	
							A 7	12: 42 41 55 39 69 72 70 86 56 40 65 50	97	6.18E+05	
							B 1	10: 43 42 41 56 57 39 85 86 69 54	98	8.52E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 2	6: 43 42 41 70 57 86	96	2.39E+05	
							B 4	4: 43 57 71 70	85	3.50E+04	
3,4,5-trimethyl-1-hexene	**56728-10-0**	**1.39**					A 1	12: 43 42 71 41 57 39 70 55 56 86 38 69	68	2.55E+06	
							A 2	13: 43 71 42 41 57 70 39 56 86 85 62 54 63	68	2.66E+06	
							A 3	3: 67 87 85	68	4.89E+06	
							A 5	8: 43 71 42 41 57 50 56 86	68	1.54E+06	
							A 7		67	6.20E+05	
							B 1	1: 70	68	2.04E+05	
							C 1	7: 85 99 71 110 98 68 39	67	2.17E+05	
γ-butyrolactone	96-48-0	1.40	Caramel, Sweet	Creamy, Oily, Fatty, Caramel			A 7	12: 42 41 55 39 69 72 70 86 56 40 65 50	71	4.33E+05	
Acrylic acid	79-10-7	1.40			2.95E-01	2.95E-01	B 1	3: 72 55 58	65	2.17E+04	7.36E+04
2,3,4-trimethylpentane	565-75-3	1.40					A 4		75	1.52E+04	
							A 7	9: 43 70 41 55 57 53 56 54 50	77	2.03E+05	
3-methylpentane	96-14-0	1.45					A 1	5: 57 56 41 58 71	98	4.98E+05	
							A 2	8: 57 56 41 71 39 58 54 85	99	5.18E+05	
							A 3		98	6.94E+05	
							A 4		87	2.06E+05	
							A 6	2: 57 39	70	3.72E+04	
							A 7		97	1.22E+05	
							B 1	6: 57 41 56 58 55 51	95	2.92E+05	
							B 2	1: 57	86	6.05E+04	
							B 4	2: 57 56	91	5.56E+04	
2-methylaziridine	75-55-8	1.45					A 1	5: 57 56 41 58 71	86	4.98E+05	
							A 2	8: 57 56 41 71 39 58 54 85	80	5.18E+05	
							A 3		81	6.94E+05	
							A 4	3: 56 41 57	77	1.54E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							A 5	5: 57 56 55 58 86	81	4.24E+05	
							A 7	5: 57 56 41 53 39	81	1.67E+05	
							B 1	6: 57 41 56 58 55 51	80	2.28E+05	
							B 2	1: 57	78	6.05E+04	
							B 4	2: 57 56	80	5.56E+04	
Isocyanatomethane	624-83-9	1.46					A 3		80	1.20E+04	
							A 4		81	5.01E+04	
							A 6	2: 57 39	80	1.03E+05	
							A 7		85	1.22E+05	
							B 1	2: 57 56	79	7.68E+03	
							B 2	2: 56 57	79	7.77E+03	
							B 4	2: 56 57	78	1.20E+03	
Cyanogen chloride	506-77-4	1.47					B 2	8: 61 63 62 97 100 35 47 37	74	1.69E+05	
1,2-dichloro-, (Z)-ethene	156-59-2	1.47				1.91E+01	B 1	4: 60 62 55 86	100	5.02E+05	2.63E+04
							B 2	6: 96 98 59 62 60 47	91	1.71E+05	8.96E+03
Furan	110-00-9	1.47		Ethereal	4.50E+03		B 2	2: 39 68	80	9.70E+03	2.16E+00
							B 4	1: 68	68	4.04E+04	8.99E+00
1,1-dichloro ethene	75-35-4	1.47			3.55E+01		B 2		99	3.57E+05	1.01E+04
Dimethylsulfide	75-18-3	1.51	Cabbage, Sulfur, Gasoline	Sulfury, Onion, Sweet corn, Vegetable, Cabbage, Tomato, Green, Radish		2.24E-03	A 2	3: 47 39 35	66	5.52E+04	2.47E+07
							A 7	5: 46 45 47 61 35	94	9.43E+04	4.21E+07
Carbon disulfide	75-15-0	1.52		Sulfur, Cabbage, Vegetable		9.55E-02	A 4	4: 76 39 86 59	82	6.35E+04	6.65E+05
							A 5	2: 44 39	84	7.99E+04	8.36E+05
3-pentanone	96-22-0	1.53	Ether	Ethereal, Acetone		3.16E-01	A 4	2: 57 86	74	9.06E+04	2.86E+05
							A 6		67	3.85E+04	1.22E+05
							B 3	2: 57 86	66	2.69E+04	8.50E+04
Butane	**106-97-8**	**1.57**				**2.04E+02**	A 1		79	3.90E+05	1.91E+03
							A 2	2: 43 58	78	5.36E+05	2.62E+03
							A 4	2: 43 42	83	1.85E+04	9.04E+01
							A 6		83	2.61E+06	1.28E+04

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 7	5: 41 59 44 37 60	84	1.88E+06	9.21E+03
							B 1	7: 43 58 42 39 37 44 60	83	2.99E+06	1.47E+04
							B 2		77	1.35E+05	6.62E+02
							B 3	6: 43 58 42 39 38 36	84	1.96E+06	9.59E+03
							B 4		87	4.62E+04	2.26E+02
							C 1		69	4.25E+04	2.08E+02
							C 2	2: 43 42	67	6.65E+04	3.26E+02
							C 3	3: 43 58 42	68	7.06E+04	3.46E+02
Hordenine	539-15-1	1.57					A 6	1: 58	66	3.41E+04	
Propanal	123-38-6	1.59	Solvent, Pungent	Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty	1.00E-02	2.69E-02	A 1	2: 58 42	76	9.76E+04	3.63E+06
							A 6		76	1.57E+04	5.85E+05
							A 7		76	3.30E+04	1.23E+06
							B 1	2: 57 58	75	7.59E+04	2.82E+06
							B 2	1: 58	73	4.63E+04	1.72E+06
							B 3	2: 58 57	77	5.57E+04	2.07E+06
							B 4	1: 58	83	1.04E+05	3.88E+06
1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide	1447-71-8	1.61					A 1	2: 58 42	75	1.50E+05	
							A 2	1: 58	73	7.42E+04	
							A 6	5: 58 38 59 52 36	71	3.95E+05	
							A 7		65	3.33E+04	
							B 1	2: 57 58	68	7.59E+04	
							B 2	1: 58	70	4.63E+04	
							B 3		71	1.40E+04	
							B 4	1: 58	68	1.24E+05	
Acetone	**67-64-1**	**1.66**		**Solvent**		**1.45E+01**	A 1	4: 43 58 42 37	97	5.84E+05	4.04E+04
							A 2	2: 43 58	96	5.36E+05	3.71E+04
							A 3	2: 43 58	81	4.96E+04	3.43E+03
							A 4		98	8.97E+05	6.20E+04
							A 6	7: 43 58 42 39 57 38 44	99	2.71E+06	1.88E+05
							A 7	10: 43 58 42 39 41 38 37 44 36 59	99	4.98E+06	3.45E+05
							B 1	7: 43 58 42 39 37 44 60	99	2.99E+06	2.07E+05
							B 2		93	1.35E+05	9.35E+03

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							B 3	6: 43 58 42 39 38 36	99	1.96E+06	1.35E+05
							B 4	10: 43 58 59 42 41 39 38 37 36 45	99	2.96E+06	2.05E+05
							C 1		87	4.25E+04	2.94E+03
							C 2	2: 43 42	90	6.65E+04	4.60E+03
							C 3	3: 43 58 42	88	7.06E+04	4.88E+03
2-methyl-2-propanamine	**75-64-9**	**1.67**					A 2	1: 58	89	7.42E+04	
							A 6	3: 60 53 36	79	9.02E+04	
							B 1	3: 42 41 55	76	9.02E+04	
							C 3	2: 58 42	70	3.20E+04	
Acetic anhydride	**108-24-7**	**1.70**		**Sharp, Vinegar**		**5.89E-01**	A 1	1: 43	66	9.90E+03	1.68E+04
							A 2	1: 43	72	2.31E+05	3.93E+05
							A 3		66	1.47E+04	2.50E+04
							A 4	2: 43 41	81	3.73E+04	6.33E+04
							A 5	5: 43 42 39 41 37	80	4.76E+05	8.09E+05
							A 6		65	2.59E+03	4.40E+03
							A 7	2: 43 85	77	5.45E+04	9.26E+04
							B 4	2: 42 43	79	8.59E+04	1.46E+05
							C 3	2: 43 41	70	3.38E+04	5.74E+04
Isobutyraldehyde	78-84-2	1.76	Pungent, Malt, Green	Spicy		4.07E-02	A 1		78	2.20E+07	5.40E+08
							A 2	13: 43 41 57 72 39 55 56 38 40 73 62 66 65	78	2.02E+07	4.96E+08
							A 3	3: 53 73 61	80	1.63E+06	3.99E+07
							A 6		73	6.15E+03	1.51E+05
							A 7		88	1.52E+04	3.73E+05
							B 1		93	3.08E+04	7.55E+05
							B 2	7: 42 41 72 53 55 56 38	77	7.00E+05	1.72E+07
							B 3		85	7.70E+03	1.89E+05
							B 4	4: 42 43 57 72	75	6.45E+04	1.58E+06
Methyl acetate	79-20-9	1.77		Ethereal			A 1		81	2.05E+04	
							A 4	1: 43	97	2.81E+05	
							A 6	7: 43 74 59 42 45 72 44	94	1.54E+06	
							B 3	5: 43 41 59 73 75	99	4.56E+05	
							B 4	4: 43 74 42 59	95	1.24E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
Cyclohexene	110-83-8	2.02				3.63E-01	A 7	2: 67 82	70	2.95E+04	8.12E+04
Methacrolein	78-85-3	2.14		Wild hyacinth foliage			A 7		87	3.42E+04	
Butyraldehyde	123-72-8	2.16	Pungent, Green	Pungent, Cocoa, Musty, Green, Malty, Bread			A 6		72	4.12E+04	
							B 1	3: 41 44 72	73	1.92E+04	
							B 3		89	2.08E+04	
							B 4		91	2.41E+04	
2-butanone	78-93-3	2.31	Ether	Ethereal, Fruity, Camphor		7.76E+00	A 4	1: 43	68	3.13E+05	4.03E+04
							A 6		79	1.13E+04	1.46E+03
2-butenal	4170-30-3	2.31		Flower		1.35E-01	A 7		79	3.42E+04	2.54E+05
2-butanone	**78-93-3**	**2.31**	**Ether**	**Ethereal, Fruity, Camphor**		**7.76E+00**	A 7	1: 43	79	2.25E+04	2.90E+03
							B 1	1: 43	76	1.16E+05	1.49E+04
							B 3	3: 72 43 127	75	3.07E+04	3.96E+03
							C 1	2: 43 72	79	1.06E+04	1.37E+03
methylhydrazine	60-34-4	2.32					A 3		79	2.05E+04	
Diazomethane	334-88-3	2.33					A 7	3: 41 42 59	71	3.00E+04	
							B 3	2: 40 42	66	1.01E+05	
Isopropyl alcohol	**67-63-0**	**2.33**		**Alcohol, Musty, Woody**		**1.02E+01**	A 1	3: 45 43 41	77	1.50E+05	1.46E+04
							A 3	2: 45 42	68	5.38E+04	5.26E+03
							A 6	3: 45 44 72	75	1.43E+05	1.40E+04
							B 3		68	7.49E+04	7.32E+03
							C 1	4: 44 90 38 37	70	6.13E+05	5.99E+04
							C 2	15: 45 57 44 47 46 42 72 56 73 39 60 89 71 38 74	65	8.30E+06	8.12E+05
							C 3	1: 45	65	1.24E+04	1.21E+03
Formic acid	64-18-6	2.33		Acetic		2.82E+01	A 1	3: 46 42 45	69	1.38E+05	4.91E+03
							A 2	1: 46	79	6.39E+04	2.27E+03
							A 3		79	4.06E+04	1.44E+03
							A 7	6: 45 46 39 42 41 47	67	4.35E+05	1.55E+04
							B 1	4: 46 45 39 42	67	1.45E+05	5.14E+03
							B 2	2: 45 46	77	4.31E+04	1.53E+03
Nitrogen dioxide	10102-44-0	2.34				1.86E-01	A 1	1: 46	76	2.63E+04	1.41E+05
							A 2	1: 46	76	4.35E+04	2.34E+05
Ethanol	64-17-5	2.34	Sweet	Alcoholic		2.88E+01	A 1		95	1.29E+05	4.47E+03
							A 2		94	1.20E+05	4.15E+03

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 3		95	7.50E+04	2.60E+03
							A 6		72	1.69E+05	5.86E+03
							A 7	6: 45 46 39 42 41 47	99	3.01E+05	1.04E+04
							B 1	4: 46 45 39 42	84	9.90E+04	3.43E+03
							B 2	2: 45 46	78	4.31E+04	1.49E+03
							B 3	4: 43 207 42 46	79	5.88E+04	2.04E+03
							B 4		92	5.54E+04	1.92E+03
Methylene chloride	75-09-2	2.42				2.82E+01	A 1	2: 86 39	94	1.76E+05	6.23E+03
							A 2	3: 51 48 47	97	2.98E+05	1.06E+04
							A 4	5: 84 51 88 42 50	97	3.88E+05	1.38E+04
							A 5	2: 47 49	98	2.81E+05	9.98E+03
							A 6		92	2.13E+04	7.56E+02
							A 7	5: 84 39 86 88 47	95	7.08E+04	2.51E+03
							B 3		91	1.67E+04	5.92E+02
							B 4	7: 84 49 88 51 47 83 48	97	1.62E+05	5.74E+03
Amitrole	61-82-5	2.44					B 4	1: 84	67	4.85E+04	
Allyl alcohol	107-18-6	2.75		Pungent, Mustard		2.69E-01	A 6		71	1.94E+04	7.19E+04
Methylbutanal	590-86-3	2.75	Malt	Ethereal, Aldehydic, Chocolate, Peach, Fatty	1.00E+00	2.24E-03	B 3		68	2.92E+04	1.30E+07
Allyl alcohol	107-18-6	2.75		Pungent, Mustard		2.69E-01	B 3		75	2.92E+04	1.08E+05
Acetonitrile	75-05-8	3.28			9.77E+01		B 1		96	1.18E+05	1.20E+03
							B 2		96	9.20E+04	9.42E+02
Chloroform	67-66-3	3.78					A 1	2: 85 83	78	3.97E+04	
							A 2		76	1.45E+04	
							A 4		79	1.70E+04	
							A 5		84	2.62E+04	
							A 6		86	2.07E+04	
							B 4	2: 83 47	79	7.69E+04	
Propyl formate	110-74-7	3.91		Sweet, Ethereal, Green, Rum, Fruity, Berry		3.39E+00	A 7	1: 42	72	1.56E+05	4.59E+04
Hydrazine	302-01-2	3.92				3.00E+00	A 1	1: 33	77	2.35E+03	7.85E+02

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 2	1: 33	77	1.56E+03	5.21E+02
							A 3	1: 33	77	9.74E+02	3.25E+02
							A 7	3: 33 45 37	77	4.44E+03	1.48E+03
							B 1	1: 33	77	3.54E+03	1.18E+03
							B 4	1: 33	76	8.26E+02	2.75E+02
3-pentanol	584-02-1	3.92	Fruit	Herbal		4.68E-01	A 1		69	1.14E+05	2.43E+05
							A 2	3: 60 59 45	68	1.06E+05	2.27E+05
							A 3		67	6.67E+04	1.43E+05
							A 7		71	1.21E+05	2.58E+05
							B 1		70	1.01E+05	2.17E+05
							B 3	3: 59 60 53	77	7.79E+05	1.67E+06
							B 4	9: 59 42 60 41 57 39 58 40 36	75	2.14E+06	4.58E+06
1,1-dimethyl-hydrazine	57-14-7	3.92					A 1	1: 42	76	6.10E+04	
							A 2	3: 60 59 45	80	1.06E+05	
							A 3	1: 42	76	1.59E+05	
							A 7		83	1.41E+05	
							B 1	2: 59 45	77	6.29E+04	
							B 3	3: 59 60 33	80	1.87E+05	
							B 4	9: 59 42 60 41 57 39 58 40 36	80	6.00E+05	
Ethylenediamine	107-15-3	3.92					A 1		79	7.94E+04	
							A 2		75	8.76E+04	
							A 3	3: 42 60 59	71	2.81E+04	
							A 7		75	1.41E+05	
							B 1		75	1.01E+05	
							B 3	3: 59 60 53	71	4.76E+05	
							B 4	7: 41 38 60 61 33 44 58	79	5.13E+05	
tert-butanol	75-65-0	3.93		Camphor			A 2		70	1.53E+04	
							B 3	3: 59 60 53	77	7.79E+05	
							B 4	9: 59 42 60 41 57 39 58 40 36	74	2.14E+06	
Methyl formate	107-31-3	3.93		Fruity, Plum		9.33E+01	A 1	1: 33	79	5.81E+03	6.22E+01
							A 4	1: 60	72	3.42E+03	3.67E+01
							B 4	7: 41 38 60 61 33 44 58	71	5.62E+05	6.02E+03
Propylamine	107-10-8	3.94		Ammoniacal		1.10E-02	A 2		76	5.74E+04	5.23E+06

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 4	9: 59 42 60 41 57 39 58 40 36	73	2.12E+06	1.94E+08
Tetrahydrofurfuryl acetate	637-64-9	4.07		Sweet, Fruity, Brown, Rum, Ether, Caramel			A 6		70	2.00E+04	
							B 3	4: 71 55 43 67	67	1.57E+04	
Phenylethyl alcohol	60-12-8	5.06	Honey, Spice, Rose, Lilac	Floral		1.70E-02	A 2		74	9.14E+04	5.38E+06
Toluene	108-88-3	5.07	Paint	Sweet		1.55E+00	A 1		81	1.39E+04	8.98E+03
							A 2		96	9.14E+04	5.90E+04
							B 1	1: 91	79	5.82E+04	3.76E+04
Pentanal	110-62-3	5.97	Almond, Malt, Pungent	Fermented		6.03E-03	B 3	3: 44 41 58	70	3.47E+04	5.76E+06
Hexanal	66-25-1	5.99	Grass, Tallow, Fat	Green	4.00E-03	1.38E-02	A 6		85	4.12E+04	2.98E+06
							A 7		84	3.44E+04	2.49E+06
							B 1	7: 43 41 72 55 45 207 82	90	1.22E+05	8.87E+06
							B 2	11: 82 44 55 41 72 39 45 43 81 58 53	94	5.45E+05	3.95E+07
							B 3		73	2.30E+04	1.66E+06
Glutaraldehyde	111-30-8	6.02					B 1		69	1.15E+05	
							B 2	11: 82 44 55 41 72 39 45 43 81 58 53	70	5.45E+05	
1-butanol	71-36-3	6.09	Medicine, Fruit	Fermented		4.90E-01	A 3	2: 56 41	79	1.25E+05	2.54E+05
							A 4		77	1.82E+04	3.72E+04
							A 6	4: 43 39 56 42	79	3.76E+04	7.67E+04
							A 7	3: 41 39 56	83	3.18E+04	6.48E+04
							B 1	3: 56 55 39	92	1.21E+05	2.47E+05
							B 2	2: 57 208	66	2.51E+05	5.12E+05
							B 3	5: 56 43 57 39 72	97	9.87E+05	2.01E+06
							B 4	12: 41 43 55 42 45 39 38 40 33 37 73 49	97	1.44E+06	2.95E+06
Butyl formate	592-84-7	6.09		Fruity			A 3	2: 56 41	67	9.56E+04	
							A 7	3: 41 39 56	65	2.32E+04	
							B 3	7: 39 43 56 40 57 41 44	82	9.78E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 4	16: 56 41 43 55 39 40 46 57 73 38 45 74 51 49 54 50	85	3.94E+06	
Isobutanol	78-83-1	6.10	Wine, Solvent, Bitter	Ethereal, Winey			B 4	2: 59 37	85	2.76E+05	
Propanoic acid, anhydride	**123-62-6**	**6.46**					A 1	1: 57	67	1.65E+03	
							A 2	1: 57	67	3.80E+03	
							A 3		68	4.04E+03	
							A 4	3: 57 85 34	68	7.52E+03	
							A 6	1: 57	76	3.42E+04	
							A 7	1: 57	68	1.34E+04	
							B 2		69	4.60E+03	
							B 3		77	1.89E+04	
							C 1	1: 57	66	3.20E+03	
							C 2	1: 57	66	4.68E+03	
							C 3	1: 57	66	8.12E+03	
4-methyl-3-penten-2-one	141-79-7	6.66	Sweet, Chemical	Pungent, Earthy, Vegetable, Acrylic		5.62E-02	B 1	2: 98 83	73	3.78E+04	6.72E+05
							B 3		94	1.03E+05	1.83E+06
							B 4	4: 55 42 63 77	97	6.77E+05	1.20E+07
2,2'-Bioxirane	1464-53-5	6.66					B 3	3: 55 51 43	65	9.31E+04	
α-angelica lactone	591-12-8	6.66					B 3	3: 55 51 43	82	1.17E+05	
Isoamyl alcohol	123-51-3	7.52	Whiskey, Malt, Burnt	Fusel oil, Alcoholic, Whiskey, Fruity, Banana		4.47E-02	A 6		73	3.77E+04	8.43E+05
							B 3		75	7.91E+04	1.77E+06
Amyl alcohol	71-41-0	7.52	Balsamic	Fusel, Oil, Sweet, Balsam		4.68E-01	A 6		78	3.77E+04	8.05E+04
							B 3		79	7.91E+04	1.69E+05
2-isopropenyl-3-methylpyrazine	145984-65-2	7.67					A 7	4: 135 75 134 133	73	1.03E+05	
α-phellandrene	**99-83-2**	**7.89**	**Turpentine, Mint, Spice**	**Terpenic**			A 1	20: 77 40 80 43 121 94 78 92 38 107 136 42 82 90 50 33 137 115 135 117	81	1.00E+07	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							A 2	5: 91 107 93 136 92	95	7.06E+05	
							A 3	6: 105 107 93 77 81 54	74	3.57E+05	
							A 5	13: 94 91 93 55 51 136 92 79 121 77 108 103 122	90	8.87E+04	
							A 6	4: 93 55 105 78	90	9.41E+04	
							A 7	11: 92 136 91 93 108 78 39 77 107 106 66	79	1.55E+06	
							B 2	20: 93 39 67 136 94 77 79 78 92 80 53 41 81 68 137 55 63 95 52 69	74	1.37E+06	
							B 3	2: 91 93	82	1.77E+04	
							B 4		85	3.25E+04	
							C 1		90	8.81E+04	
							C 2		86	3.75E+04	
							C 3	7: 136 93 91 92 103 77 94	89	8.42E+04	
α-pinene	**80-56-8**	**7.90**	**Pine, Turpentine**	**Herbal**		**6.92E-01**	A 1	12: 79 93 106 91 78 41 136 51 94 92 77 67	93	1.05E+06	1.52E+06
							A 2		97	6.09E+06	8.80E+06
							A 3	10: 93 91 121 77 43 81 106 94 39 53	92	2.14E+05	3.09E+05
							A 5	8: 93 81 68 107 43 105 95 78	93	3.65E+05	5.28E+05
							A 6		93	1.61E+05	2. 33E+05
							A 7	11: 92 136 91 93 108 78 39 77 107 106 66	97	4.88E+05	7.05E+05
							B 1	11: 92 81 78 39 41 65 107 281 80 122 69	98	1.79E+06	2.58E+06

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 2	20: 93 39 67 136 94 77 79 78 92 80 53 41 81 68 137 55 63 95 52 69	98	1.24E+06	1.79E+06
							B 3		88	9.49E+04	1.37E+05
							B 4		83	3.25E+04	4.69E+04
							C 1		71	5.23E+04	7.56E+04
							C 2		75	3.75E+04	5.42E+04
							C 3	7: 136 93 91 92 103 77 94	70	8.42E+04	1.22E+05
Betahistine	5638-76-6	7.90					A 1	3: 65 74 104	65	2.02E+07	
							A 3		69	4.37E+04	
							A 4		67	1.03E+04	
							A 5	8: 136 93 80 43 41 106 65 94	70	5.56E+05	
							A 6	6: 136 94 79 106 93 121	73	4.42E+05	
							A 7		68	5.61E+05	
							B 1	18: 77 79 68 80 53 52 121 136 106 105 43 41 64 51 103 66 81 54	67	1.29E+06	
Conessine	546-06-5	8.31					B 3	2: 71 84	69	5.94E+03	
							B 4	1: 84	74	5.31E+04	
2-formyl pyrrole	**1003-29-8**	**9.09**		**Musty, Beefy, Coffee**			C 3	3: 95 94 81	67	7.92E+03	
1,4-dimethoxybenzene	**150-78-7**	**9.19**		**Sweet, Green, New mown hay, Fennel**			C 1		67	1.39E+04	
							C 2		66	2.81E+04	
α-ionol	**25312-34-9**	**9.20**		**Ionone, Tropical, Sweet, Floral, Violet, Woody**			C 1		73	2.42E+04	
							C 3	7: 138 95 82 80 55 45 140	68	1.92E+05	
Menthyl acetate	**16409-45-3**	**9.20**				**6.17E+00**	C 1	5: 138 94 123 95 79	74	1.46E+05	2.37E+04

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors		Published ODT (ppm)		Code	Models	Net % Match	PAC	OAV
			Flavornet[1]	TGSC[2]	LRI & Odour[3]	Devos, *et al.*[4]					
				Tea cooling, Minty, Fruity, Berry			C 2	2: 138 96	79	5.85E+04	9.49E+03
							C 3		77	2.29E+04	3.71E+03
4-methyl guaiacol	**93-51-6**	**9.20**		**Spicy**			C 1	5: 138 94 123 95 79	74	1.18E+05	
2-acetyl-6-methyl pyrazine	**22047-26-3**	**9.26**		**Roasted coffee, Cocoa, Popcorn**			B 3	3: 93 136 41	70	1.67E+04	
							C 2	15: 93 136 39 80 94 78 67 108 102 104 120 38 75 54 49	65	3.00E+07	
Tricyclene	508-32-7	9.30					A 2	6: 136 133 92 78 107 40	81	3.13E+05	
							A 6	6: 136 94 79 106 93 121	71	4.42E+05	
2-indanone	615-13-4	9.47					B 1	6: 104 77 103 39 51 102	66	1.82E+05	
Styrene	100-42-5	9.48	Balsamic, Gasoline	Balsamic		1.45E-01	B 1	6: 104 77 103 39 51 102	97	1.82E+05	1.26E+06
							B 2		81	2.19E+04	1.52E+05
β-pinene	18172-67-3	9.90	Pine, Resin, Turpentine	Terpenic			A 1	11: 136 52 128 81 119 78 90 56 83 59 55	96	2.64E+07	
							A 2	18: 69 41 79 53 39 94 67 80 70 107 66 51 117 137 52 104 37 59	97	1.09E+07	
							A 3		93	7.03E+05	
							A 4		67	2.39E+04	
							A 5	5: 69 93 121 51 94	80	5.33E+05	
							A 6		73	8.95E+05	
							A 7		92	5.61E+05	
							B 1	20: 93 69 41 91 39 68 51 92 79 136 77 67 65 94 53 54 107 82 137 52	96	3.92E+06	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 2	20: 69 53 77 78 39 94 121 70 55 42 68 65 89 67 52 40 51 105 66 56	95	5.72E+06	
							B 3		75	3.51E+04	
Myrcene	123-35-3	9.94	Balsamic, Must, Spice	Peppery, Terpene, Spicy, Balsam, Plastic	1.30E-02		A 1	12: 41 92 43 120 80 40 53 51 55 79 52 78	88	1.86E+06	1.43E+08
							A 2	1: 38	92	1.36E+06	1.05E+08
							A 3	12: 93 81 41 94 77 43 91 121 70 79 51 106	94	1.37E+06	1.05E+08
							A 5		92	2.88E+05	2.22E+07
							A 7		94	6.11E+05	4.70E+07
							B 1	20: 93 69 41 91 39 68 51 92 79 136 77 67 65 94 53 54 107 82 137 52	97	3.92E+06	3.02E+08
							B 2	20: 69 53 77 78 39 94 121 70 55 42 68 65 89 67 52 40 51 105 66 56	96	5.72E+06	4.40E+08
							B 3	3: 93 92 41	71	3.05E+04	2.34E+06
DL-menthol	**89-78-1**	**10.34**		**Peppermint, Cool, Woody**	**4.17E-02**		C 1		67	1.01E+05	2.42E+06
							C 3	7: 138 95 82 80 55 45 140	66	6.55E+04	1.57E+06
(±)-menthol	**1490-04-6**	**10.34**		**Minty**		**4.17E-02**	C 1		70	1.01E+05	2.42E+06
							C 2	9: 95 138 139 96 94 67 109 123 68	70	1.39E+05	3.34E+06
							C 3		69	1.90E+05	4.56E+06
o-dimethyl hydroquinone	**91-16-7**	**10.34**		**Vanilla**			C 3	9: 95 94 138 96 123 67 53 81 79	69	3.63E+05	
(+)-carvomenthene	**1195-31-9**	**10.34**					C 1		85	1.01E+05	
							C 2		85	8.21E+04	
							C 3		86	1.90E+05	
Menthol	**15356-70-4**	**10.36**			**4.17E-02**		C 3		66	8.02E+04	1.92E+06

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
2,4,6-trimethylphenol	**527-60-6**	**10.48**		**Phenolic**			C 1	6: 57 39 107 135 116 52	82	4.11E+05	
α-terpinene	**99-86-5**	**10.50**	**Lemon**	**Woody**			A 1	3: 121 75 68	66	1.37E+06	
							A 2	20: 136 121 93 91 79 77 105 39 51 41 64 120 53 107 106 55 95 50 40 116	96	4.75E+06	
							A 7	13: 121 78 136 68 103 117 80 52 51 77 106 107 81	80	2.20E+05	
							B 1	3: 136 91 107	78	4.82E+04	
							C 1	20: 136 93 53 91 78 41 107 122 137 77 79 105 92 119 50 39 65 108 115 90	97	2.04E+06	
							C 2		97	1.40E+06	
							C 3	20: 91 93 79 107 136 92 106 77 95 65 89 51 43 108 137 94 102 68 115 50	98	1.71E+06	
(+)-4-Carene	**29050-33-7**	**10.50**			**4.00E+00**		A 1	7: 93 119 121 137 53 105 136	94	3.68E+05	9.21E+04
							A 2	20: 136 121 93 91 79 77 105 39 51 41 64 120 53 107 106 55 95 50 40 116	99	4.75E+06	1.19E+06
							A 3		91	3.19E+04	7.97E+03
							A 5	5: 105 119 121 80 136	67	7.28E+04	1.82E+04
							A 7	13: 121 78 136 68 103 117 80 52 51 77 106 107 81	82	2.20E+05	5.49E+04
							B 1		84	2.29E+04	5.73E+03

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							C 1	20: 136 93 53 91 78 41 107 122 137 77 79 105 92 119 50 39 65 108 115 90	98	2.04E+06	5.10E+05
							C 2		98	1.40E+06	3.50E+05
							C 3	20: 121 136 122 103 78 77 105 80 41 106 107 39 43 94 120 115 52 135 67 54	98	1.10E+06	2.74E+05
Furfurylmethylamphetamine	13445-60-8	10.50					A 1	1: 81	73	5.34E+04	
Phenylacetic acid	103-82-2	10.53	Honey, Flower	Sweet, Honey, Floral, Honeysuckle, Sour, Waxy, Civet			A 2	3: 91 136 43	70	7.97E+04	
1-hexanol	111-27-3	10.73	Resin, Flower, Breen	Herbal		4.37E-02	A 6		87	5.03E+04	1.15E+06
Diacetone alcohol	123-42-2	10.78				8.91E-01	A 7	2: 59 43	77	5.51E+04	6.18E+04
							B 3		87	2.54E+05	2.85E+05
							B 4	9: 43 59 101 39 83 55 61 40 45	92	1.75E+06	1.96E+06
(1R)-(+)-trans-isolimonene	5113-87-1	10.85					B 4	8: 79 121 136 105 94 95 108 81	71	6.65E+04	
2,2,5-trimethylhexane	3522-94-9	10.88					A 4	4: 56 57 71 136	80	1.28E+05	
Limonene	**138-86-3**	**10.89**	**Lemon, Orange**	**Citrus**	**1.00E-02**	**4.37E-01**	A 1	20: 92 105 80 51 117 66 137 122 62 81 64 54 104 63 76 108 103 134 38 43	95	3.33E+07	7.64E+07
							A 2	20: 68 93 67 94 136 59 107 91 53 39 81 95 105 55 65 66 119 137 52 96	95	2.21E+07	5.05E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

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Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 3	20: 68 79 93 67 107 115 94 92 77 63 136 39 80 41 91 108 69 95 54 137	95	1.97E+06	4.51E+06
							A 4	20: 68 92 93 41 67 39 57 71 65 77 55 79 85 94 53 136 91 56 121 191	82	4.35E+05	9.97E+05
							A 6	8: 92 67 93 65 136 80 107 39	87	2.06E+05	4.71E+05
							A 7	6: 68 92 80 136 69 41	90	1.71E+05	3.92E+05
							B 1		95	2.16E+06	4.94E+06
							B 2		95	1.71E+06	3.93E+06
							B 3		90	1.76E+05	4.03E+05
							B 4	3: 67 121 77	76	8.21E+04	1.88E+05
							C 1	16: 93 67 69 107 39 121 92 136 52 122 41 137 42 77 55 51	93	3.17E+05	7.26E+05
							C 2	7: 68 91 136 67 121 65 69	87	1.62E+05	3.71E+05
							C 3		80	3.86E+04	8.84E+04
Camphene	**79-92-5**	**10.93**	**Camphor**	**Woody**			A 1	20: 92 105 80 51 117 66 137 122 62 81 64 54 104 63 76 108 103 134 38 43	89	3.33E+07	
							A 2	20: 68 93 67 94 136 59 107 91 53 39 81 95 105 55 65 66 119 137 52 96	89	2.21E+07	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 3	20: 68 79 93 67 107 115 94 92 77 63 136 39 80 41 91 108 69 95 54 137	89	1.97E+06	
							A 4	20: 68 92 93 41 67 39 57 71 65 77 55 79 85 94 53 136 91 56 121 191	78	4.35E+05	
							A 5	12: 91 53 67 65 121 107 80 105 93 77 41 95	87	4.38E+05	
							A 6	8: 92 67 93 65 136 80 107 39	82	2.06E+05	
							A 7	7: 79 68 136 107 92 95 91	84	1.33E+05	
							B 1		90	2.16E+06	
							B 2		90	1.71E+06	
							B 3		85	1.76E+05	
							B 4	8: 79 121 136 105 94 95 108 81	79	3.71E+04	
							C 1		88	2.97E+05	
							C 2	11: 93 94 120 51 122 77 65 104 108 52 103	65	2.52E+05	
							C 3		82	8.67E+07	
Eucalyptol	470-82-6	10.97	Mint, Sweet	Eucalyptus, Herbal, Camphor		1.62E-02	A 6		80	1.58E+05	9.75E+06
							B 3		70	1.03E+05	6.36E+06
N-Benzyl-2-phenethylamine	3647-71-0	11.32					B 3	2: 120 91	75	1.22E+04	
Phenyl propane	103-65-1	11.32					B 3	2: 120 91	70	1.22E+04	
3-ethyl-o-xylene	933-98-2	11.35					A 2	13: 91 119 78 77 105 55 103 50 104 120 135 133 63	81	8.85E+05	
m-cymene	**535-77-3**	**11.36**					A 1		96	3.98E+05	
							A 2		98	1.76E+06	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

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Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 3	2: 119 91	73	3.59E+04	
							A 4	2: 119 65	71	4.21E+04	
							A 6		92	4.31E+04	
							A 7		86	3.49E+04	
							B 1		91	5.27E+04	
							B 3	3: 119 91 134	93	9.48E+04	
							C 1	19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130	99	6.79E+07	
							C 2		99	3.74E+07	
							C 3	20: 119 134 91 77 135 93 92 51 78 116 58 50 128 52 86 87 129 101 131 126	97	3.94E+07	
p-cymene	**99-87-6**	**11.36**	**Solvent, Gasoline, Citrus**	**Terpenic**		**2.14E-03**	A 1		93	3.98E+05	1.86E+08
							A 2		95	1.76E+06	8.22E+08
							A 3	1: 119	74	5.38E+04	2.52E+07
							A 4	2: 119 65	70	5.56E+04	2.60E+07
							A 6		91	4.31E+04	2.01E+07
							A 7		85	3.49E+04	1.63E+07
							B 1		89	5.27E+04	2.46E+07
							B 3	3: 119 91 134	91	9.48E+04	4.44E+07
							C 1	19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130	97	6.79E+07	3.18E+10
							C 2		97	3.74E+07	1.75E+10
							C 3	20: 119 134 91 77 135 93 92 51 78 116 58 50 128 52 86 87 129 101 131 126	93	3.94E+07	1.84E+10
	488-23-3	**11.36**				**2.63E-02**	A 1		91	3.98E+05	1.51E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

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Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
1,2,3,4-tetramethylbenzene							A 2	14: 119 134 117 118 39 135 103 89 116 133 41 78 64 51	94	1.33E+06	5.06E+07
							A 3	2: 134 119	72	4.73E+04	1.80E+06
							A 4	3: 119 117 63	67	2.58E+04	9.82E+05
							A 5	2: 119 134	67	8.39E+03	3.19E+05
							A 6	5: 119 134 120 117 57	86	1.25E+05	4.77E+06
							A 7		80	3.49E+04	1.33E+06
							B 1		85	5.27E+04	2.00E+06
							B 3	3: 119 91 134	87	9.48E+04	3.60E+06
							C 1	19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130	95	6.79E+07	2.58E+09
							C 2		95	3.74E+07	1.42E+09
							C 3	20: 119 134 91 77 135 93 92 51 78 116 58 50 128 52 86 87 129 101 131 126	93	3.94E+07	1.50E+09
1-ethyl-2,4-dimethylbenzene	874-41-9	11.36					A 1	5: 93 78 119 104 106	76	1.24E+05	
							A 3	1: 119	78	5.38E+04	
							A 4	2: 119 65	72	5.56E+04	
							A 6	5: 119 134 120 117 57	84	1.23E+05	
							B 1	3: 134 120 77	79	7.74E+04	
							B 3	2: 119 120	76	6.36E+04	
1-phenyl-1-decanone	6048-82-4	11.40					A 2	6: 57 63 117 58 120 105	71	2.12E+05	
N,N-dimethylbenzenamine	121-69-7	11.40					A 2	6: 57 63 117 58 120 105	71	2.12E+05	
Isodurene	**527-53-7**	**11.40**					A 1	3: 57 119 134	79	2.50E+04	
							A 2	4: 119 39 134 193	75	3.12E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 4	3: 119 117 63	69	2.60E+04	
							B 1	2: 119 134	67	7.78E+04	
							C 1	20: 119 134 91 105 103 104 39 75 128 50 53 52 90 76 38 94 106 114 85 98	77	5.94E+07	
1-(3-methylphenyl)-ethanone	585-74-0	11.41					A 1	5: 93 78 119 104 106	83	7.20E+04	
							A 3	2: 119 91	71	3.59E+04	
							B 1	3: 91 120 134	76	6.51E+04	
Dihydromethylcyclopentapyrazine	**23747-48-0**	**11.41**	**Roast, Nut**	**Earthy, Baked potato, Peanut, Roasted**			A 1	3: 57 119 134	75	1.56E+05	
							A 2	4: 119 39 134 193	69	3.12E+04	
							C 1	19: 64 90 106 76 59 49 133 128 66 85 107 129 101 126 113 67 73 111 130	70	2.87E+07	
1-ethyl-3,5-dimethylbenzene	**934-74-7**	**11.46**					A 2	8: 134 119 116 117 62 102 57 71	68	3.87E+05	
							C 1	20: 119 134 91 105 103 104 39 75 128 50 53 52 90 76 38 94 106 114 85 98	82	6.16E+07	
Methylisohexenyl ketone	110-93-0	11.51	Pepper, Mushroom, Rubber	Citrus		3.80E-02	A 4		93	3.18E+05	8.35E+06
							A 6	9: 52 68 65 57 45 77 54 84 50	98	4.30E+06	1.13E+08
							A 7		80	4.51E+04	1.19E+06
							B 3	4: 65 70 82 97	98	3.30E+06	8.67E+07
							B 4	7: 93 108 67 117 55 68 126	94	3.97E+05	1.04E+07
4-ethyl-1,2-dimethylbenzene	934-80-5	11.57					A 2	8: 134 119 116 117 62 102 57 71	67	3.91E+05	
δ-3-carene	**13466-78-9**	**11.57**	**Lemon, Resin**	**Citrus**	**4.00E+00**		A 1	4: 108 91 43 105	78	7.76E+04	1.94E+04
							A 2	8: 134 119 116 117 62 102 57 71	97	3.80E+06	9.51E+05
							A 3		90	7.79E+04	1.95E+04

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 5	9: 107 93 92 136 80 118 65 120 79	71	3.01E+05	7.53E+04
							A 6		73	9.13E+05	2.28E+05
							A 7	19: 92 79 94 105 95 91 148 63 65 204 120 41 123 82 135 78 66 39 128	70	1.42E+06	3.56E+05
							B 1	11: 137 79 93 136 92 107 94 77 78 81 53	96	3.24E+05	8.11E+04
							B 2	7: 79 43 67 51 136 40 105	75	3.15E+05	7. 88E+04
							B 3		72	8.48E+05	2.12E+05
							B 4		71	2.10E+05	5.25E+04
							C 1	4: 90 41 122 107	85	9.59E+06	2.40E+06
							C 2	10: 106 122 108 138 135 94 64 68 82 63	90	2.21E+06	5.52E+05
							C 3	20: 91 93 79 107 136 92 106 77 95 65 89 51 43 108 137 94 102 68 115 50	72	1.82E+06	4.54E+05
Sabinene	3387-41-5	11.59	Pepper, Turpentine, Wood	Woody			A 1	20: 77 40 80 43 121 94 78 92 38 107 136 42 82 90 50 33 137 115 135 117	79	9.81E+06	
							A 2	11: 136 105 92 67 79 43 68 94 51 106 138	88	1.53E+06	
							A 3		90	7.79E+04	
							A 7	7: 91 67 107 108 41 94 63	69	1.09E+05	
							B 1	18: 77 79 68 80 53 52 121 136 106 105 43 41 64 51 103 66 54 81	75	1.30E+06	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
γ-terpinene	**99-85-4**	**11.79**	**Gasoline, Turpentine**	**Terpenic**			A 2		85	5.28E+04	
							A 7	7: 77 107 80 121 92 137 63	69	1.64E+05	
							C 1	14: 91 136 105 79 78 53 76 80 137 55 81 75 68 127	98	1.32E+08	
							C 2	18: 91 79 43 107 119 51 103 117 66 55 88 74 135 129 42 123 101 87	99	1.25E+08	
							C 3	16: 93 91 121 105 41 43 63 122 52 81 76 102 38 42 127 120	99	8.67E+07	
Terpinolene	**586-62-9**	**11.83**	**Pine, Plastic**	**Herbal**	**2.00E-01**		A 1	11: 136 52 128 81 119 78 90 56 83 59 55	73	3.87E+06	1.94E+07
							A 2	20: 136 121 93 91 79 77 105 39 51 41 64 120 53 107 106 55 95 50 40 116	90	6.01E+06	3.00E+07
							A 3		87	3.19E+04	1.59E+05
							C 1	3: 137 67 104	82	4.17E+05	2.09E+06
							C 2	18: 91 79 43 107 119 51 103 117 66 55 88 74 135 129 42 123 101 87	95	1.25E+08	6.26E+08
							C 3	16: 93 91 121 105 41 43 63 122 52 81 76 102 38 42 127 120	95	8.67E+07	4.33E+08
Ethyl benzene	**100-41-4**	**11.84**				**2.88E+00**	C 1	14: 91 136 105 79 78 53 76 80 137 55 81 75 68 127	67	9.64E+07	3.34E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							C 2	18: 91 79 43 107 119 51 103 117 66 55 88 74 135 129 42 123 101 87	71	7.80E+07	2.70E+07
Acetic acid	64-19-7	12.23	Sour	Acidic		1.45E-01	A 6	8: 43 60 45 42 41 44 40 59	100	2.76E+07	1.91E+08
							A 7	3: 43 44 207	100	7.66E+05	5.30E+06
							B 1	3: 45 43 60	90	1.91E+04	1.32E+05
							B 3	4: 43 45 60 42	98	1.62E+07	1.12E+08
N-methyl-N-nitroso urea	684-93-5	12.26					A 7	4: 43 60 42 44	70	1.71E+05	
(z)-rose oxide	**16409-43-1**	**12.28**		**Green, Red rose, Spic, Fresh geranium**			C 2	14: 69 139 96 97 83 70 95 55 140 207 154 67 71 66	66	2.19E+05	
							C 3	4: 139 140 96 84	68	2.25E+05	
Phenetole	103-73-1	12.52					A 2	7: 122 107 68 51 50 94 117	70	1.18E+05	
2-hydroxyacetophenone	**118-93-4**	**12.53**		**Phenolic**			A 1		86	7.20E+04	
							A 2	5: 136 107 137 93 122	85	7.49E+04	
							A 3		80	1.89E+04	
							A 4	2: 121 136	75	5.91E+04	
							A 6	2: 121 136	74	9.22E+03	
							A 7	7: 43 136 121 81 92 53 91	67	2.20E+04	
							C 1	13: 121 93 41 122 136 67 55 108 106 92 104 53 94	78	8.16E+05	
1-methyl-2-propyl benzene	**1074-17-5**	**12.63**					C 1	2: 134 105	73	1.91E+04	
2-phenyl propionaldehyde	**93-53-8**	**12.63**		**Fresh, Sharp, Green, Hyacinth, Leaf, Lilac**			C 1	2: 134 105	66	1.91E+04	
o-xylene	95-47-6	13.07	Geranium	Geranium		8.51E-01	A 2	5: 77 134 106 119 52	73	9.60E+04	1.13E+05

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
p-xylene	106-42-3	13.08				4.90E-01	A 2		81	4.01E+04	8.19E+04
4-methylphenethylamine	3261-62-9	13.08					A 2		69	4.01E+04	
2,3-dimethyl-cyclohexanol	1502-24-5	13.19					B 3		68	1.94E+04	
Fenchone	**1195-79-5**	**13.47**				**9.33E-02**	A 6	6: 81 69 152 53 80 67	95	2.96E+05	3.17E+06
							B 3	4: 41 39 109 77	91	1.41E+05	1.51E+06
							C 1	19: 81 41 53 55 79 39 82 91 80 137 67 70 42 105 123 85 38 153 77	98	1.36E+06	1.46E+07
							C 2	13: 153 152 80 55 77 78 91 42 71 66 52 40 123	99	1.43E+06	1.53E+07
							C 3	20: 81 69 152 67 80 41 66 68 82 39 109 72 91 52 55 137 97 42 153 40	98	1.50E+06	1.60E+07
Linalool oxide	5989-33-3	13.67	Flower, Wood	Earthy, Floral, Sweet, Woody			A 5	11: 207 266 83 70 79 55 112 67 85 53 97	65	1.91E+05	
							A 6		83	8.06E+04	
							A 7	19: 93 55 111 70 92 71 94 43 67 81 83 68 91 69 84 74 57 137 82	80	3.23E+05	
							B 3	5: 111 81 71 95 93	82	8.43E+04	
1,3-diethylbenzene	141-93-5	13.81					A 2	14: 105 93 94 137 81 53 65 119 77 120 82 135 51 39	68	3.70E+05	
2-ethylhexanol	104-76-7	13.81	Rose, Green	Citrus		2.45E-01	A 5		87	1.48E+05	6.05E+05
							A 6		85	9.88E+04	4.03E+05
							A 7	7: 84 41 54 112 43 56 70	91	3.39E+05	1.38E+06

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 1	3: 82 56 71	95	5.55E+05	2.26E+06
							B 3	4: 83 71 57 41	92	1.23E+05	5.01E+05
							B 4		66	2.31E+04	9.39E+04
Methyl vinyl ketone	78-94-4	13.82		Sweet			A 6	4: 70 55 39 82	67	1.34E+04	
Tranylcypromine	155-09-9	13.91					A 2	7: 132 117 102 118 91 115 99	69	1.31E+06	
Propanoic acid	79-09-4	13.91	Pungent, Rancid, Soy	Pungent, Acidic, Cheesy, Vinegar		3.55E-02	A 6	3: 73 74 60	65	1.76E+05	4.97E+06
5-methylindane	**874-35-1**	**13.91**					A 1		88	2.94E+05	
							A 2	5: 132 116 39 131 57	90	1.91E+06	
							B 1	5: 91 132 115 116 64	78	4.44E+04	
							C 1	5: 132 115 131 65 91	75	1.10E+05	
2-ethenyl-1,3-dimethylbenzene	**2039-90-9**	**13.91**					A 1		92	2.94E+05	
							A 2	7: 132 117 102 118 91 115 99	94	1.31E+06	
							B 1	5: 91 132 115 116 64	82	4.44E+04	
							C 1	5: 132 115 131 65 91	82	1.10E+05	
Propylene glycol	**57-55-6**	**13.98**					A 1	3: 45 43 41	72	1.50E+05	
							A 2		68	1.20E+05	
							A 3		67	7.50E+04	
							A 7	6: 45 46 39 42 41 47	71	3.01E+05	
							B 3		72	4.64E+04	
							B 4	2: 42 43	67	7.41E+04	
							C 1	4: 44 90 38 37	69	6.13E+05	
							C 2	17: 45 43 47 44 55 90 76 53 73 115 71 41 60 56 51 54 40	69	6.30E+06	
Indane	496-11-7	13.98					A 1	3: 118 115 117	68	1.10E+05	
	532-27-4	14.09				2.57E-02	A 5	6: 105 51 77 52 78 63	78	6.57E+05	2.56E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
2-chloroacetophenone							A 7		76	1.00E+06	3.89E+07
							B 1	3: 77 78 50	76	3.34E+05	1.30E+07
							B 2		71	2.25E+04	8.76E+05
							B 3	3: 105 106 107	71	1.30E+05	5.06E+06
							B 4	6: 105 77 106 78 51 107	74	1.07E+05	4.17E+06
Benzaldehyde	100-52-7	14.09	Almond, Burnt sugar	Fruity	3.00E-03	4.17E-02	A 5		98	8.98E+05	2.15E+07
							A 7		98	1.00E+06	2.40E+07
							B 1	3: 77 78 50	97	5.17E+05	1.24E+07
							B 2	3: 106 105 77	83	4.03E+04	9.66E+05
							B 3	3: 105 106 107	89	1.30E+05	3.12E+06
							B 4	6: 105 77 106 78 51 107	93	1.07E+05	2.57E+06
Ethyl lactate	**97-64-3**	**14.10**	**Fruit**	**Sharp, Tart, Fruity, Buttery, Butterscotch**		**1.62E+00**	A 6	4: 45 46 75 47	87	2.84E+05	1.75E+05
							B 3	4: 43 207 42 46	84	5.88E+04	3.63E+04
							C 1	10: 72 90 56 73 37 60 74 48 71 76	80	9.99E+06	6.16E+06
							C 2	12: 72 39 56 73 41 71 60 53 49 52 48 40	80	6.67E+06	4.11E+06
							C 3	13: 55 42 58 41 60 56 38 73 91 54 89 74 132	79	1.64E+07	1.01E+07
Isobutyrophenone	611-70-1	14.10		Green			B 1	3: 77 78 50	69	3.34E+05	
Dimethyl octanol	**106-21-8**	**14.11**		**Waxy, Soapy, Aldehydic, Leathery, Musty, Citrus, Green**			C 1	8: 54 70 111 67 97 56 53 110	82	7.44E+05	
							C 2	6: 70 41 57 79 84 97	66	2.13E+05	
1-Dodecanol	**112-53-8**	**14.11**	**Fat, Wax**	**Earthy, Soapy, Waxy, Fatty, Honey, Coconut**		**1.26E-02**	C 1		93	2.64E+05	2.10E+07
							C 2	6: 70 41 57 79 84 97	76	1.91E+05	1.52E+07
1-Decanol	**112-30-1**	**14.11**	**Fat**			**1.82E-02**	C 1		75	6.38E+04	3.51E+06

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
				Fatty, Waxy, Floral, Orange, Sweet, Clean, Watery			C 2	6: 70 41 57 79 84 97	86	7.90E+04	4.34E+06
1-Nonanol	**143-08-8**	**14.12**	**Fat, Green**	**Fresh, Clean, Fatty, Floral, Rose, Orange, Dusty, Wet, Oily**	**5.00E+01**	**2.24E-03**	C 1 C 2		76 71	3.03E+04 7.50E+04	1.35E+07 3.35E+07
Undecane	**1120-21-4**	**14.13**	**Alkane**			**1.17E+00**	C 1	7: 85 99 71 110 98 68 39	68	2.43E+05	2.07E+05
Nonane	**111-84-2**	**14.13**	**Alkane**	**Gasoline**		**1.26E+00**	C 1	7: 85 99 71 110 98 68 39	77	2.17E+05	1.72E+05
Dodecane	**112-40-3**	**14.13**	**Alkane**	**Alkane**		**2.04E+00**	C 1	7: 85 99 71 110 98 68 39	77	2.17E+05	1.06E+05
Tridecane	**629-50-5**	**14.14**	**Alkane**	**Alkane**		**2.14E+00**	A 4 C 1	 7: 85 99 71 110 98 68 39	68 68	1.59E+04 2.43E+05	7.44E+03 1.14E+05
2,2-dimethylbutane	75-83-2	14.15					A 4		82	1.59E+04	
3-isopropyl phenol	**618-45-1**	**14.19**					A 1	7: 121 77 55 136 67 120 79	77	3.82E+05	
							A 2	7: 122 105 103 93 121 51 57	82	7.66E+05	
							C 3	20: 121 136 122 103 78 77 105 80 41 106 107 39 43 94 120 115 52 135 67 54	81	1.39E+06	
3-(1-methylethyl)-phenol methylcarbamate	64-00-6	14.20					A 1	8: 121 105 136 106 91 77 79 265	76	7.43E+05	
							A 2	13: 105 121 51 79 136 77 78 53 103 106 39 120 43	74	7.94E+05	
							A 4	2: 136 121	65	6.07E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							A 7	13: 121 78 136 68 103 117 80 52 51 77 106 107 81	66	3.18E+05	
							B 1	3: 136 91 107	74	4.44E+04	
Acetone cyanohydrin	75-86-5	14.27					B 1	4: 70 83 112 69	69	3.20E+04	
							B 3	1: 70	70	8.97E+03	
1,4-diethylbenzene	105-05-5	14.47					A 1		87	9.45E+04	
							A 2	9: 120 55 115 93 135 52 108 103 133	85	5.16E+05	
o-cymene	527-84-4	14.47				7.94E-04	A 2	18: 91 52 119 106 134 93 55 105 92 115 103 117 79 65 120 63 133 116	88	4.83E+05	6.08E+08
1,2-diethylbenzene	135-01-3	14.47					A 1		85	9.45E+04	
							A 2	18: 91 52 119 106 134 93 55 105 92 115 103 117 79 65 120 63 133 116	84	8.70E+05	
p-tert-butylphenol	98-54-4	14.48		Leathery			A 7		68	1.54E+04	
tert-butyl-benzene	98-06-6	14.48					A 1		89	6.59E+04	
							A 2		86	3.38E+05	
							B 1	3: 91 120 134	76	6.51E+04	
o-methylacetophenone	577-16-2	14.48		Floral		6.61E-03	A 1		89	6.59E+04	9.98E+06
2-methoxyethanol	109-86-4	14.62					A 6	2: 43 55	65	1.39E+05	
2-Butanol	**78-92-2**	**14.66**	**Wine**	**Sweet, Apricot**	**1.70E+00**		C 3	13: 45 43 47 44 55 46 42 54 60 58 76 38 86	69	2.96E+07	1.74E+07
Maltol	118-71-8	14.67	Caramel	Sweet, Caramel, Cotton candy, Jam, Fruity, Baked bread			A 4	3: 98 126 71	66	5.65E+03	
Linalyl acetate	115-95-7	15.09	Sweet, Fruit	Herbal		8.91E-03	A 4		77	2.39E+04	2.68E+06
							A 6	1: 83	74	4.56E+04	5.12E+06

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
Geranyl butyrate	106-29-6	15.09	Fruit, Rose, Apple	Sweet, Fruity, Rose, Waxy Raspberry, Tropical			A 4		68	1.45E+04	
Isobornyl thiocyanoacetate	115-31-1	15.11					A 1	20: 92 105 80 51 117 66 137 122 62 81 64 54 104 63 76 108 103 134 38 43	66	3.33E+07	
							A 2	20: 68 93 67 94 136 59 107 91 53 39 81 95 105 55 65 66 119 137 52 96	66	2.21E+07	
							A 3	9: 81 137 95 106 122 43 42 108 103	67	9.69E+05	
							A 6	20: 55 65 77 93 39 41 136 80 43 81 121 86 139 97 53 94 91 52 105 84	70	7.74E+05	
							A 7	20: 93 69 80 71 72 122 41 92 55 107 136 65 94 53 81 105 45 56 96 82	68	3.68E+05	
							B 3	10: 72 139 94 65 70 57 67 92 52 54	73	1.18E+06	
Linalyl propionate	144-39-8	15.11		Fresh, Bergamot, Lily, Woody, Rose, Rum			B 3	17: 121 93 41 82 80 94 70 67 105 68 84 51 56 53 72 137 126	67	6.45E+05	
Linalool	78-70-6	15.12	Flower, Lavender	Floral	6.00E-03	5.37E-02	A 1	3: 69 71 43	85	9.62E+04	1.79E+06
							A 2		89	1.00E+05	1.87E+06
							A 5		91	3.31E+05	6.16E+06
							A 6		96	8.95E+05	1.67E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							A 7	20: 93 69 80 71 72 122 41 92 55 107 136 65 94 53 81 105 45 56 96 82	95	3.68E+05	6.85E+06
							B 3	10: 72 139 94 65 70 57 67 92 52 54	97	1.18E+06	2.19E+07
Ethyl cyclohexane	**1678-91-7**	**15.17**					C 1	6: 55 83 84 67 169 139	71	3.95E+05	
1-methyl-1H-imidazole	**616-47-7**	**15.20**					C 3	3: 82 69 168	67	1.48E+05	
cis-2-pinanol	4948-29-2	15.41		Herbal			A 5		72	1.30E+04	
							A 6	20: 81 99 79 97 121 67 77 43 68 83 95 71 86 72 94 108 107 69 57 105	95	8.31E+05	
							A 7		79	1.66E+04	
							B 3	4: 94 93 58 72	92	5.15E+05	
trans-carveol	**1197-07-5**	**15.51**	**Caraway, Solvent**	**Caraway, Solvent, Spearmint**			C 1	19: 109 106 43 137 67 119 69 39 134 65 79 94 110 41 82 105 117 115 121	74	1.36E+06	
β-cyclocitral	**432-25-7**	**15.52**	**Mint**	**Tropical, Saffron, Herbal, clean, Rose, Sweet, Tobacco, Damascenone, Fruity**			C 1		87	1.15E+06	
							C 2	20: 95 134 119 138 77 106 121 152 137 67 107 41 79 65 91 78 117 120 110 55	87	9.49E+05	
							C 3		86	8.54E+05	
tetrahydro-2-methyl-2-furanol	**7326-46-7**	**15.57**					C 1	7: 71 43 72 78 39 41 82	76	2.27E+05	
Fenchyl alcohol	1632-73-1	15.72	Camphor	Camphor, Borneol, Pine,			A 1		76	4.88E+04	
							A 2	2: 80 81	67	7.96E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
				Woody, Dry, Sweet, Lemon			A 4	12: 81 107 43 41 83 72 71 69 121 53 96 67	92	2.37E+05	
							A 5		78	5.65E+04	
							A 6	20: 81 107 72 84 41 69 55 111 92 71 93 123 121 83 122 57 43 95 79 77	98	1.84E+06	
							A 7		72	1.94E+04	
							B 3		99	2.28E+06	
							B 4		83	2.67E+04	
1-methyl-1H-pyrrole	96-54-8	15.72		Smoky, Woody, Herbal			A 2	3: 81 80 69	69	2.65E+04	
(-)-terpinen-4-ol	20126-76-5	16.20					A 6		70	1.45E+04	
1-terpinen-4-ol	562-74-3	16.20	Turpentine, Nutmeg, Must	Woody, Ceding, mentholic, Citrus, Terpiny, Spicy			A 6		74	1.45E+04	
Thujone	**546-80-5**	**16.22**		**Cedar leaf**		**1.29E-01**	C 3		72	8.49E+03	6.59E+04
2-Methyl-4-(1-methylethyl)-2-cyclohexenone	**41469-46-9**	**16.33**					C 1	4: 109 81 95 65	77	5.92E+04	
							C 2		80	3.89E+04	
							C 3		82	3.07E+04	
Camphor	**76-22-2**	**16.33**	**Camphor**	**Camphorous**	**5.13E-02**		C 2		69	3.89E+04	7.58E+05
							C 3		69	6.43E+04	1.25E+06
Pulegone	**89-82-7**	**16.34**		**Peppermint, Camphor, Fresh, Herbal, Buchu**	**3.39E-03**		C 1	4: 152 67 109 81	71	6.25E+04	1.85E+07
							C 2		76	3.90E+04	1.15E+07
2,2,4-trimethylpentane	540-84-1	16.57					A 4	6: 57 99 56 140 183 86	77	3.93E+05	
γ-hexalactone	695-06-7	17.20	Coumarin, Sweet	Tonka			B 3	1: 85	78	3.62E+04	
Borneol	507-70-0	17.60	Camphor	Pine, Woody, Camphor		2.09E-03	A 6	6: 139 77 110 92 94 91	96	8.39E+05	4.01E+08
							B 3		98	7.46E+05	3.57E+08

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
Isobornyl acetate	125-12-2	17.60		Balsamic			A 6	6: 139 77 110 92 94 91	77	8.39E+05	
							B 3		79	7.46E+05	
Laevo-borneol	464-45-9	17.60		Pine, Woody, Camphor			A 6		95	4.15E+05	
							B 3	19: 95 69 121 79 105 140 55 67 92 68 43 110 70 91 111 108 42 57 113	98	6.63E+05	
α-terpineol	98-55-5	17.73	Oil, Anise, Mint	Floral		3.72E-02	A 1		84	6.15E+04	1.66E+06
							A 2		80	3.85E+04	1.04E+06
							A 4		83	3.03E+04	8.17E+05
							A 5		80	3.75E+04	1.01E+06
							A 6		94	7.72E+05	2.08E+07
							A 7		80	2.54E+04	6.84E+05
							B 3		95	5.95E+05	1.60E+07
α-terpinyl acetate	80-26-2	17.73	Wax	Herbal, Bergamot, Lavender, Lime, Citrus			A 3	20: 121 136 68 93 41 77 94 51 52 54 78 43 95 80 69 65 42 119 63 103	67	1.20E+06	
							A 4	2: 136 121	68	4.41E+04	
							A 5	7: 136 80 93 95 41 43 81	77	6.84E+04	
							B 1	6: 136 92 63 119 80 66	69	4.56E+05	
Terpinyl butyrate	2153-28-8	17.74		Sour, Rosemary, Fruity, Balsam			A 7	4: 136 94 68 93	68	1.57E+04	
2-ethyl-3,5-dimethylpyridine	1123-96-2	17.91					A 1	4: 68 82 134 133	66	1.28E+05	
							B 1	2: 134 135	74	2.22E+04	
p-cresyl acetate	140-39-6	18.14		Narcissus, Phenolic, Animal		7.76E-04	A 7	1: 108	65	9.23E+03	1.19E+07
m-tert-butylphenol	585-34-2	18.15					A 7	5: 135 80 108 79 91	68	6.76E+04	
Verbenone	80-57-9	18.16					A 5		75	9.46E+03	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
				Camphor, Menthol, Celery			A 7		82	2.55E+04	
1-Tetradecanol	**112-72-1**	**18.32**	**Coconut**	**Fruity, Waxy, Orris, Coconut**			C 1		80	8.39E+04	
3-methylhexane	**589-34-4**	**18.32**					A 4		72	1.66E+04	
							C 1	10: 57 98 82 71 68 43 67 56 70 127	75	3.62E+04	
1-Tridecene	**2437-56-1**	**18.33**					C 2		80	4.71E+04	
1-undecanol	**112-42-5**	**18.34**	**Mandarin**	**Waxy**		**6.76E-02**	C 1		74	6.38E+04	9.44E+05
							C 2	6: 70 41 57 79 84 97	82	7.90E+04	1.17E+06
Octyl formate	**112-32-3**	**18.34**		**Fruity, rose, Orange, Waxy, Cucumber**			C 2		67	1.25E+04	
α-copaene	3856-25-5	18.39	Wood, Spice	Wood			A 1		71	3.09E+04	
α-cubebene	17699-14-8	18.50	Herb, Wax	Herb			A 1		73	1.57E+04	
(+)-sativene	3650-28-0	19.40					A 1		78	5.89E+04	
							A 5	20: 93 69 120 148 106 68 55 92 189 95 149 175 135 162 190 136 83 91 53 103	75	2.37E+07	
Nitro cyclohexane	**1122-60-7**	**19.46**					C 2	2: 83 55	67	2.04E+04	
β-caryophyllene	87-44-5	19.66	Wood, Spice	Spice	6.40E-02		A 1	20: 133 69 79 161 105 120 136 81 77 106 119 162 121 39 109 94 175 92 82 123	100	6.01E+06	9.40E+07
							A 2	17: 189 106 92 41 148 190 81 80 93 78 95 121 77 161 94 91 120	99	2.39E+06	3.73E+07
							A 3		77	3.32E+04	5.19E+05
							A 4		80	3.35E+04	5.24E+05

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							A 6	20: 41 133 93 69 107 147 148 120 66 55 121 80 42 176 119 95 53 43 145 136	99	4.19E+06	6.55E+07
							A 7	10: 134 124 96 66 112 190 122 110 177 138	89	1.05E+06	1.64E+07
							B 3		99	3.11E+06	4.86E+07
							B 4	14: 94 69 120 135 107 163 80 78 134 176 161 109 63 82	99	1.37E+06	2.14E+07
Benzyl alcohol	100-51-6	19.74	Sweet, Flower	Floral			A 5	11: 78 53 109 149 39 129 66 65 123 134 202	96	2.16E+07	
							A 7		96	5.83E+06	
							B 1	13: 108 79 78 51 91 109 90 39 86 62 92 74 37	100	3.59E+06	
							B 2	11: 108 107 77 80 76 106 49 91 105 53 41	99	8.86E+05	
Tyramine	51-67-2	19.74		Meaty			A 5	6: 51 85 38 62 90 75	70	9.20E+06	
							A 7	5: 90 62 109 37 61	70	3.71E+06	
							B 1	1: 53	70	4.00E+06	
							B 2		72	6.78E+05	
α-guaiene	3691-12-1	19.85	Wood, Balsamic	Wood			A 1		80	2.88E+05	
							A 2	13: 106 189 133 123 162 93 204 95 120 108 94 205 105	91	5.50E+05	
							A 5		72	3.36E+05	
							A 6	16: 107 147 108 93 94 106 91 67 105 189 121 81 51 69 119 53	94	4.50E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							B 3		94	3.21E+05	
							B 4	13: 107 204 135 79 133 119 105 147 81 148 73 65 95	88	9.51E+04	
Dimethylsulfone	67-71-0	20.12	Sulfur, Burnt	Sulfurous, Burnt			A 7	2: 94 79	80	1.93E+04	
δ-cadinene	483-76-1	20.20	Thyme, Medicine, Wood	Herbal			A 1	20: 161 204 190 122 39 202 107 55 65 134 41 159 69 81 149 67 109 53 78 117	66	4.74E+05	
							A 5		74	1.51E+04	
2,6-pyridinediamine	141-86-6	20.49					A 5	1: 109	71	4.03E+03	
α-humulene	6753-98-6	20.53	Wood	Wood	1.20E-01		A 1	19: 147 93 121 67 92 105 81 109 39 80 91 119 77 57 41 43 135 103 120	97	1.68E+06	1.40E+07
							A 2		91	1.76E+05	1.47E+06
							A 5	20: 93 80 121 107 79 92 147 91 70 41 105 109 205 94 122 189 106 82 204 95	98	3.99E+06	3.32E+07
							A 6	20: 107 105 80 67 190 109 94 95 106 147 92 41 68 83 189 108 65 52 42 205	96	1.55E+06	1.29E+07
							A 7	19: 92 79 94 105 95 91 148 63 65 204 120 41 123 82 135 78 66 39 128	97	1.42E+06	1.19E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 3	20: 121 93 107 148 91 106 123 66 39 122 42 175 204 95 205 40 73 120 133 129	97	1.47E+06	1. 23E+07
							B 4		93	2.10E+05	1.75E+06
β-selinene	17066-67-0	21.25	Herb	Herb			A 1		93	3.35E+05	
							A 2		86	6.14E+04	
							A 6	14: 161 135 108 119 163 81 94 109 105 78 41 93 82 149	92	3.26E+05	
							A 7	15: 161 162 134 94 190 43 91 81 204 121 123 95 92 131 175	72	1.56E+05	
							B 3		92	1.84E+05	
							B 4		85	4.15E+04	
Longifolene	475-20-7	21.27		Wood			A 1	20: 133 69 79 161 105 120 136 81 77 106 119 162 121 39 109 94 175 92 82 123	89	6.01E+06	
							A 2	17: 189 106 92 41 148 190 81 80 93 78 95 121 77 161 94 91 120	89	2.39E+06	
							A 5	17: 147 205 68 133 161 148 189 105 175 93 107 135 109 123 53 69 134	91	6.66E+05	
							A 6	20: 41 133 93 69 107 147 148 120 66 55 121 80 42 176 119 95 53 43 145 136	90	4.19E+06	
							A 7		87	1.16E+05	
							B 3		90	3.11E+06	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
							B 4	14: 94 69 120 135 107 163 80 78 134 176 161 109 63 82	88	1.37E+06	
Alloaromadendrene	25246-27-9	21.41	Wood	Wood			B 3	20: 55 135 96 121 79 93 105 161 148 106 204 120 91 80 127 94 77 122 205 104	71	1.21E+06	
α-bulnescene	3691-11-0	21.41					A 2		89	1.96E+05	
							A 6	6: 105 136 69 43 42 109	94	1.08E+06	
							B 3	20: 55 135 96 121 79 93 105 161 148 106 204 120 91 80 127 94 77 122 205 104	96	1.07E+06	
							B 4		92	4.36E+05	
α-gurjunene	489-40-7	21.43	Wood, Balsamic	Wood			A 1		85	2.68E+05	
							A 2		73	1.22E+04	
							A 5		88	2.34E+05	
							A 6	3: 145 147 109	82	2.85E+05	
							A 7	10: 147 131 107 133 109 204 119 79 95 105	81	1.34E+05	
							B 3		81	5.86E+04	
							B 4	9: 106 119 51 149 162 161 123 81 117	81	3.10E+04	
Aromadendrene	489-39-4	21.48	Wood	Wood			A 1		65	6.94E+04	
							A 2	8: 82 93 147 121 162 67 65 133	73	1.48E+05	
							A 5		71	8.73E+04	
							A 6		81	5.80E+04	
							A 7		91	1.16E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 3	19: 161 147 105 129 133 204 106 109 95 77 145 82 92 91 108 190 120 41 117	87	9.66E+04	
2,4,6-trimethylpyridine	108-75-8	21.66					A 2	4: 121 67 39 106	65	1.24E+05	
							A 6		72	1.01E+04	
Phenol	108-95-2	21.68	Phenolic	Phenolic		1.10E-01	B 1		78	1.73E+04	1. 58E+05
Dyclocaine	586-60-7	21.69					A 1		70	6.94E+04	
(-)-Aristolene	6831-16-9	21.74					A 1	15: 108 119 79 135 204 189 133 187 106 148 67 55 42 43 78	74	4.92E+05	
							A 6		81	5.14E+04	
							B 3	11: 161 204 79 148 107 53 109 81 202 108 105	83	8.64E+04	
2-ethylphenol	90-00-6	21.91		Phenolic			A 5	2: 122 107	71	3.34E+03	
(+)-calarene	17334-55-3	22.08					A 1	20: 121 91 107 162 95 105 189 81 136 135 134 79 39 110 92 57 190 53 160 146	73	2.22E+06	
							A 2		71	2.89E+04	
							A 5	17: 147 109 161 91 148 204 135 133 92 189 107 94 93 159 134 41 149	78	6.42E+05	
							A 6	17: 161 121 122 149 136 67 189 55 135 81 145 162 148 39 80 41 134	70	8.30E+05	
							B 3	16: 148 105 161 162 205 92 67 133 107 79 135 115 134 120 93 119	78	1.44E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 4	20: 77 147 161 67 134 189 65 121 105 133 82 95 55 79 120 109 43 83 108 78	73	6.04E+05	
α-cedrene	469-61-4	22.08		Woody, Cedar, Sweet, Fresh			A 5	15: 119 204 161 93 65 69 133 80 121 135 134 41 189 94 79	72	4.47E+05	
							A 7		72	1.74E+04	
Longicyclene	1137-12-8	22.10					A 5	17: 109 93 189 190 80 131 133 204 55 121 115 79 105 145 82 107 135	78	1.57E+05	
							B 4	7: 134 189 81 204 161 106 78	72	3.50E+05	
γ-gurjunene	22567-17-5	22.14		Musty			A 1	20: 121 91 107 162 95 105 189 81 136 135 134 79 39 110 92 57 190 53 160 146	92	2.49E+06	
							A 2		84	6.30E+04	
							A 5	20: 93 147 77 105 129 108 79 189 119 81 91 135 106 175 131 145 205 51 95 109	92	4.50E+06	
							A 6	18: 161 204 108 105 205 107 122 81 55 53 109 148 39 92 79 77 162 106	89	9.02E+05	
							A 7		89	5.08E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 3	20: 161 122 107 149 204 105 109 205 95 65 79 55 135 134 77 141 91 41 92 108	91	7.69E+05	
							B 4	20: 148 79 161 107 95 145 204 67 93 120 105 122 41 91 106 162 205 108 39 150	90	4.49E+05	
α-longipinene	5989-08-2	22.18					A 6	20: 93 121 122 204 133 115 119 135 91 205 117 105 77 159 176 54 95 162 51 163	70	1.01E+06	
Cedryl acetate	77-54-3	22.18		Wood			B 4	17: 119 105 204 69 55 190 149 107 67 96 95 205 175 106 187 147 109	65	2.31E+05	
Valencene	4630-07-3	22.19	Green, Oil	Citrus			A 1	20: 133 121 161 92 204 79 107 91 119 52 190 81 93 55 78 53 115 131 206 129	96	3.06E+06	
							A 2		88	1.47E+05	
							A 5	20: 161 204 131 133 91 53 106 190 68 108 43 66 77 94 162 78 148 73 160 143	96	3.46E+06	
							A 6	16: 134 78 135 108 204 147 161 39 82 95 79 119 107 175 52 131	95	1.39E+06	
							A 7		95	8.47E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							B 3	20: 161 91 204 133 145 78 135 81 134 79 55 119 120 63 93 53 107 108 174 122	96	1.14E+06	
							B 4	20: 77 147 161 67 134 189 65 121 105 133 82 95 55 79 120 109 43 83 108 78	94	4.66E+05	
2-hydroxyethyl acrylate	5951-61-1	22.61					A 1		79	2.64E+04	
							A 2		77	2.03E+04	
							A 5		82	6.28E+04	
							A 6	4: 133 119 109 161	79	5.29E+04	
							A 7	13: 107 121 149 81 79 42 189 190 82 161 39 136 97	73	2.79E+05	
							B 3		80	4.60E+04	
							B 4	20: 148 79 161 107 95 145 204 67 93 120 105 122 41 91 106 162 205 108 39 150	77	7.39E+05	
Butylated Hydroxytoluene	128-37-0	22.66		Mild, Phenolic, Camphor			B 1		84	3.39E+04	
							B 2		90	7.76E+04	
Xylazine	7361-61-7	22.67					B 2		66	7.76E+04	
2,3,6-trimethylpyridine	1462-84-6	23.95					A 2	5: 41 134 120 121 83	65	1.78E+04	
Toluene-2,4-diamine	95-80-7	23.97					A 2	4: 122 121 105 96	70	1.18E+04	
Propofol	2078-54-8	23.97		Phenolic			A 1	20: 93 164 108 107 178 80 124 135 79 106 122 145 41 120 55 94 91 103 95 149	68	7.95E+05	
							A 2		70	1.43E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 9 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
1-(3,6-Dimethyl-2-pyrazinyl)-2-methyl-1-propanone	145984-66-3	23.98					A 2	14: 108 123 93 67 163 81 178 107 105 91 79 66 55 145	68	1.38E+05	
Methyl isoeugenol	93-16-3	23.98	Clove, Spice	Spice			A 1	14: 163 41 93 108 107 105 119 115 91 149 95 145 78 160	67	1.50E+06	
							A 2		66	1.43E+05	
Caryophyllene oxide	1139-30-6	24.09	Herb, Sweet, Spice	Woody			A 5		74	2.69E+04	
p-acetanisole	**100-06-1**	**24.58**		**Anisic**			C 1	2: 135 150	68	1.31E+04	
							C 3		69	6.11E+03	
3-methyl-5-(1-methylethyl)-Phenol methylcarbamate	**2631-37-0**	**24.64**					C 1	2: 135 150	70	1.31E+04	
							C 2		84	2.37E+04	
							C 3	1: 150	73	2.09E+04	
Carvacrol	**499-75-2**	**24.78**		**Spicy**		**1.12E-02**	C 1		92	4.48E+04	3.99E+06
Thymol	**89-83-8**	**24.78**		**Herbal**		**1.55E-02**	C 1		91	4.48E+04	2.89E+06
							C 2		82	2.37E+04	1.53E+06
							C 3		70	6.20E+03	4.00E+05
Carvacrol	**499-75-2**	**24.78**		**Spicy**		**1.12E-02**	C 2		84	2.37E+04	2.11E+06
							C 3		72	6.20E+03	5.53E+05
2,4-di-tert-butylphenol	96-76-4	26.36		Phenolic			A 4	1: 191	68	2.90E+04	
α-bisabolol	72691-24-8	26.43					A 5		77	3.95E+04	
Cyclobarbital	52-31-3	35.80					A 7	1: 207	65	9.20E+03	
1,4-Dioxane	123-91-1	38.37				5.50E+00	B 3	2: 58 88	71	2.39E+03	4.34E+02

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Marijuana.

SI Table 10. Summary of VOCs emitted from all illicit cocaine samples and Sigma Pseudo™ Narcotic Scent Cocaine formulation over 1 hour at room temperature. Sigma Pseudo™ Narcotic Scent Cocaine formulation is indicated by underlined and **bolded** fonts.

SI Table 10 ~~continued~~

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
Ethylene oxide	**75-21-8**	**1.07**				**8.51E+02**	D 4		66	3.83E+06	4.50E+03
							E 1		66	2.28E+06	2.68E+03
2-nitropropane	79-46-9	1.11				7.24E+00	D 2	4: 41 43 56 39	88	2.92E+04	4.03E+03
							D 4		73	3.05E+04	4.21E+03
							D 5	3: 39 43 41	83	4.84E+03	6.69E+02
2,4-dimethylpentane	108-08-7	1.16				8.71E+01	D 1	4: 57 85 43 99	70	1.41E+05	1.62E+03
							D 3	5: 53 100 70 86 57	83	8.33E+05	9.57E+03
							D 4	4: 43 56 42 84	69	1.90E+04	2.18E+02
1,2-dimethyl hydrazine	540-73-8	1.18					D 1	1: 45	74	1.91E+04	
Ethylenimine	151-56-4	1.20					D 2	4: 43 42 56 41	68	7.08E+04	
Isobutane	75-28-5	1.24				1.00E+01	D 1	6: 43 42 41 57 72 39	83	1.26E+06	1.26E+05
							D 2	9: 43 42 41 57 39 55 56 53 58	84	1.43E+06	1.43E+05
							D 3	11: 43 42 41 57 72 56 55 39 38 71 51	85	3.13E+06	3.13E+05
							D 4	4: 43 42 41 72	82	2.27E+05	2.27E+04
							D 5	7: 41 43 42 39 72 57 55	81	1.53E+05	1.53E+04
Ethyl Chloride	75-00-3	1.26					D 1	2: 64 66	75	1.37E+04	
Butane	106-97-8	1.26				2.04E+02	D 1	6: 43 58 42 41 37 45	82	4.20E+06	2.06E+04
							D 2	4: 41 43 56 39	79	2.92E+04	1.43E+02
							D 4		91	3.05E+04	1.49E+02
							D 5	3: 43 56 58	87	5.11E+04	2.50E+02
Trichloromonofluoromethane	75-69-4	1.27					D 2	2: 103 101	77	5.39E+03	
Acetaldehyde	75-07-0	1.28	Pungent, Ether	Pungent, Ethereal,	1.50E-02	1.86E-01	D 1	2: 44 43	81	3.01E+04	1.61E+05
							D 2	1: 44	81	2.68E+04	1.44E+05
							D 4	3: 44 43 42	91	6.31E+04	3.39E+05

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
				Aldehydic, Fruity			D 5		68	2.60E+03	1.40E+04
Ethyl ether	60-29-7	1.31		Ethereal			D 4	2: 59 45	86	1.43E+04	
Isoprene	78-79-5	1.33					D 4	2: 53 67	82	2.29E+04	
4-methyldecane	2847-72-5	1.39					D 1	4: 56 57 55 43	72	7.44E+04	
							D 2	8: 43 71 70 41 86 55 57 56	65	5.04E+05	
							D 3	13: 70 56 71 113 99 85 41 69 67 42 72 44 114	84	8.36E+05	
							D 4	2: 42 70	65	2.98E+05	
2-methylpentane	107-83-5	1.39					D 1	2: 57 70	97	3.19E+05	
							D 2	8: 43 71 70 41 86 55 57 56	98	5.04E+05	
							D 3	6: 43 71 42 39 55 56	97	5.78E+05	
							D 4	2: 42 70	96	2.98E+05	
							D 5	6: 41 43 71 70 55 39	96	2.07E+05	
2,3-dimethylbutane	79-29-8	1.40					D 3	3: 42 41 43	65	2.60E+05	
							D 4	9: 43 71 41 39 55 86 42 53 72	87	2.93E+05	
Hexane	110-54-3	1.44	Alkane			2.19E+01	D 1	2: 43 42	96	1.06E+05	4.83E+03
							D 2	4: 43 42 56 41	83	7.76E+04	3.55E+03
							D 3	9: 57 43 41 56 86 39 58 55 70	99	2.29E+06	1.05E+05
							D 4		90	4.09E+05	1.87E+04
							D 5	4: 57 56 41 86	90	3.60E+05	1.64E+04
Cyclopentane	287-92-3	1.45		Petroleum			D 4	3: 55 70 53	77	3.85E+04	
							D 5	2: 42 55	83	2.96E+04	
2-methylaziridine	75-55-8	1.45					D 1	3: 56 41 57	80	7.68E+04	
							D 2		81	7.80E+04	
							D 3	1: 57	79	1.35E+05	
							D 4		81	6.54E+04	
							D 5		82	5.43E+04	
3-methylpentane	**96-14-0**	**1.45**					D 1	3: 56 41 57	87	7.68E+04	
							D 2		93	7.80E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							D 3	1: 57	87	1.35E+05	
							D 4		96	6.37E+04	
							D 5	2: 56 55	92	1.57E+05	
							E 1	2: 56 57	67	3.48E+03	
Isocyanatomethane	**624-83-9**	**1.46**					D 1	4: 56 57 55 43	66	8.44E+04	
							D 3	5: 57 112 85 43 113	80	8.15E+04	
							D 5	2: 56 55	80	1.23E+05	
							E 1	2: 56 57	79	3.48E+03	
2-hydroxy propanenitrile	78-97-7	1.48					D 3	9: 43 56 42 53 55 87 54 85 50	73	8.86E+05	
							D 5	2: 56 55	65	8.32E+04	
3,4,5-trimethyl-1-hexene	56728-10-0	1.51					D 1	9: 43 71 42 56 41 70 57 39 38	67	3.11E+05	
							D 2	8: 43 71 70 41 86 55 57 56	67	5.04E+05	
							D 3		69	4.99E+05	
							D 4	2: 42 70	68	2.98E+05	
							D 5	3: 43 57 71	68	1.72E+05	
Propanal	123-38-6	1.57	Solvent, Pungent	Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty	1.00E-02	2.69E-02	D 1	3: 58 57 41	68	1.47E+04	5.46E+05
Acetic anhydride	**108-24-7**	**1.62**		**Sharp, Vinegar**		**5.89E-01**	D 1	2: 61 43	69	2.06E+05	3.50E+05
							D 3	1: 43	81	3.68E+04	6.25E+04
							D 4	3: 43 58 42	81	3.40E+04	5.77E+04
							D 5	2: 43 42	73	4.76E+03	8.08E+03
							E 1	1: 43	65	1.08E+03	1.83E+03
2,2,4,4-tetramethyl-3-pentanone	815-24-7	1.65					D 1	4: 57 85 43 99	68	1.41E+05	
							D 3	5: 112 57 85 41 55	75	1.28E+05	
2-methyl-2-propanamine	75-64-9	1.65					D 4	4: 41 57 37 85	91	1.22E+05	
2,2,4,4-tetramethyl-3-pentanone	815-24-7	1.65					D 4	4: 41 57 37 85	73	3.53E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
Acetone	**67-64-1**	**1.66**		**Solvent**		**1.45E+01**	D 1	6: 43 58 42 41 37 45	99	4.20E+06	2.91E+05
							D 2	2: 43 58	88	1.55E+05	1.07E+04
							D 3	3: 58 43 42	88	9.15E+04	6.33E+03
							D 4	3: 43 58 39	97	9.33E+05	6.46E+04
							D 5	6: 43 58 57 42 37 44	97	5.36E+05	3.71E+04
							E 1	2: 58 43	81	1.03E+04	7.11E+02
Methyl acetate	79-20-9	1.68		Ethereal			D 1	1: 43	85	1.36E+05	
							D 4	3: 43 74 39	95	1.69E+05	
							D 5	3: 74 43 42	95	1.98E+05	
Acrolein	107-02-8	1.71		Almond, Cherry		1.74E-01	D 3	1: 56	66	6.09E+04	3.50E+05
Propene	115-07-1	1.71				5.25E+01	D 3	3: 41 39 42	77	3.28E+04	6.25E+02
Methacrylic anhydride	760-93-0	1.71					D 3	3: 41 39 42	75	2.28E+04	
Isobutyraldehyde	78-84-2	1.76	Pungent, Malt, Green	Spicy		4.07E-02	D 1		91	4.35E+04	1.07E+06
							D 2	9: 43 42 41 57 39 55 56 53 58	77	1.43E+06	3.50E+07
							D 3	11: 43 42 41 57 72 56 55 39 38 71 51	78	3.13E+06	7.68E+07
							D 4	4: 43 42 41 72	76	2.27E+05	5.57E+06
							D 5	7: 41 43 42 39 72 57 55	75	1.53E+05	3.77E+06
1-(ethenyloxy)-butane	111-34-2	1.89					D 3	5: 53 100 70 86 57	69	6.85E+05	
2,4-Pentanedione	123-54-6	1.91				3.16E-02	D 4		69	1.34E+04	4.25E+05
Mefruside	7195-27-9	1.91					D 4		71	1.34E+04	
Cyclohexane	**110-82-7**	**1.92**				**2.19E+01**	D 3		82	4.27E+04	1.95E+03
							D 4		89	5.25E+04	2.40E+03
							D 5	3: 55 42 41	86	3.56E+04	1.63E+03
							E 1	2: 41 84	76	1.34E+04	6.13E+02
2,3,4-trimethylpentane	565-75-3	1.98					D 3	5: 70 57 39 55 84	74	4.45E+05	
(S)-2-propylpiperidine	**458-88-8**	**1.99**					E 1		66	3.60E+03	
2-ethyl-1-butanol	97-95-0	2.00		Sweet, Musty, Alcoholic		2.34E-01	D 4	3: 84 70 39	75	1.29E+05	5.52E+05
							D 5		74	3.28E+04	1.40E+05

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
Cyclohexanone	108-94-1	2.17		Minty, Acetone		7.08E-01	D 4	4: 41 55 98 72	65	9.49E+03	1.34E+04
Nimorazole	6506-37-2	2.19					D 3	1: 100	72	8.60E+03	
2-(diethylamino)-1-phenyl-1-propanone	90-84-6	2.19					D 3	1: 100	66	8.60E+03	
Heptane	142-82-5	2.22	Alkane	Sweet, Ethereal		9.77E+00	D 3	12: 43 71 41 100 56 55 70 54 39 42 85 40	98	1.40E+06	1.43E+05
2-methyl-3-pentanone	565-69-5	2.22	Mint	Mint			D 4	3: 100 57 41	67	1.24E+04	
1,2-diethyl hydrazine	1615-80-1	2.31					D 4	6: 88 70 89 73 87 60	73	5.77E+05	
Ethylacetate	141-78-6	2.31	Pineapple	Ethereal, Fruity,		2.63E+00	D 1	9: 43 61 70 73 62 71 60 89 55	99	3.08E+06	1.17E+06
				Sweet, Weedy,			D 3	6: 61 70 73 62 90 60	99	4.00E+06	1.52E+06
				Green			D 4	10: 43 61 42 70 88 45 73 62 87 41	99	3.29E+06	1.25E+06
							D 5	7: 70 88 73 42 74 62 59	99	2.31E+06	8.80E+05
2-butanone	78-93-3	2.33	Ether	Ethereal, Fruity, Camphor		7.76E+00	D 3	4: 43 61 45 60	75	4.36E+06	5.61E+05
							D 4	3: 72 57 39	67	2.54E+05	3.27E+04
							D 5	5: 43 61 45 73 89	76	2.23E+06	2.88E+05
Methyl thiocyanate	556-64-9	2.33	Sulfur	Sulfury, Onion		1.55E-01	D 5	4: 42 73 46 60	66	3.15E+05	2.03E+06
Ethanol	64-17-5	2.34	Sweet	Alcoholic		2.88E+01	D 1	2: 45 73	87	4.09E+05	1.42E+04
							D 2		98	1.58E+05	5.47E+03
Isopropyl alcohol	67-63-0	2.34		Alcohol, Musty, Woody		1.02E+01	D 2	1: 45	81	2.69E+05	2.63E+04
							D 4		80	5.72E+05	5.59E+04
							D 5		82	2.92E+05	2.86E+04
Formic acid	64-18-6	2.34		Acetic		2.82E+01	D 1	2: 45 73	78	1.00E+06	3.56E+04
							D 2		70	8.70E+04	3.09E+03
Nitrogen dioxide	10102-44-0	2.34				1.86E-01	D 1	1: 46	75	1.36E+05	7.28E+05
							D 5	2: 46 47	76	6.16E+03	3.31E+04
methylhydrazine	60-34-4	2.35					D 1	1: 46	78	1.95E+05	
							D 2	2: 45 46	77	9.05E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
Acetic acid ethenyl ester	108-05-4	2.41					D 5	1: 86	68	8.39E+04	
Methylene chloride	75-09-2	2.41				2.82E+01	D 3	4: 84 49 48 35	97	2.87E+05	1.02E+04
							D 4	6: 84 49 86 51 35 47	93	2.60E+05	9.24E+03
							D 5	6: 49 44 57 84 48 35	93	1.22E+05	4.34E+03
Tolycaine	3686-58-6	2.43					D 5	3: 86 47 35	67	2.41E+04	
2-Pentanone	107-87-9	2.43	Ether, Fruit	Sweet, Fruity, Ethereal, Wine, Banana, Woody		1.55E+00	D 5	4: 86 49 84 43	72	6.97E+04	4.50E+04
Amitrole	61-82-5	2.49					D 3	3: 84 46 57	79	2.35E+04	
Piperoxan	59-39-2	2.60					D 3	5: 98 85 84 69 82	67	3.15E+04	
Methyl cyclohexane	108-87-2	2.61					D 3	5: 83 56 41 69 39	94	1.24E+05	
							D 4	5: 98 55 83 82 56	84	1.14E+05	
							D 5	4: 83 69 82 55	75	2.64E+04	
n-Propyl acetate	109-60-4	2.68	Fruit, Apple, Banana	Solvent, Celery, Fruity, Fusel, Raspberry, Pear		5.75E-01	D 1	9: 43 61 70 73 62 71 60 89 55	69	4.99E+06	8.68E+06
							D 3	9: 41 33 59 60 39 72 57 74 35	97	6.43E+06	1.12E+07
							D 4	10: 43 61 42 70 88 45 73 62 87 41	69	3.29E+06	5.71E+06
							D 5	7: 70 88 73 42 74 62 59	69	2.31E+06	4.02E+06
1-Heptanol	111-70-6	2.77	Chemical, Green	Musty, Leafy, Violet, Herbal, Green, Sweet, Woody, Peony		2.51E-02	D 3		73	3.82E+04	1.52E+06
Ethanedinitrile	460-19-5	3.00					D 5	2: 52 61	74	1.75E+03	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
Benzene	71-43-2	3.02		Aromatic		3.63E+00	D 1		93	1.32E+05	3.64E+04
							D 3	4: 78 50 77 79	74	2.71E+04	7.47E+03
2,5-dimethyl hexane	592-13-2	3.17					D 3	6: 70 53 43 39 99 56	84	9.76E+05	
3-methylheptane	589-81-1	3.35					D 3		93	1.29E+05	
Sorbic Acid	110-44-1	3.56					D 3		67	6.14E+04	
Isothiocyanato methane	556-61-6	3.76		Pungent, Mustard, Horseradish			D 3	4: 73 40 72 63	67	9.72E+05	
Chloroform	67-66-3	3.77					D 4	4: 83 48 61 85	79	2.12E+05	
							D 5		79	7.16E+04	
Ethylenediamine	107-15-3	3.93					D 1		68	9.65E+04	
1,1-dimethyl-hydrazine	57-14-7	3.95					D 1	3: 59 42 60	74	2.19E+04	
							D 2		79	4.75E+04	
3-pentanol	584-02-1	3.95	Fruit	Herbal		4.68E-01	D 2		66	4.75E+04	1.02E+05
Hydrazine	302-01-2	3.96				3.00E+00	D 1		79	1.44E+04	4.79E+03
							D 2	1: 33	77	1.47E+03	4.89E+02
							D 3	1: 33	78	8.97E+04	2.99E+04
							D 4	2: 111 33	78	6.05E+03	2.02E+03
Octane	111-65-9	4.00	Alkane	Gasoline		5.75E+00	D 3		91	1.90E+05	3.30E+04
Tetrahydrofurfuryl acetate	637-64-9	4.07		Sweet, Fruity, Brown, Rum, Ether, Caramel			D 3	2: 71 39	77	1.98E+05	
Isobutyl acetate	110-19-0	4.86	Fruit, Apple, Banana	Sweet, Fruity, Ethereal, Banana, Tropical		4.79E-01	D 1		91	2.03E+05	4.24E+05
Isobutyric acid	79-31-2	4.88	Rancid, Butter, Cheese			1.95E-02	D 1	2: 43 41	72	2.84E+05	1.46E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
Toluene	108-88-3	5.05	Paint	Sweet		1.55E+00	D 3	16: 91 65 93 89 39 50 38 62 77 43 45 74 90 61 46 88	100	5.76E+06	3.72E+06
Phenylethyl alcohol	60-12-8	5.05	Honey, Spice, Rose, Lilac	Floral		1.70E-02	D 3	16: 91 65 93 89 39 50 38 62 77 43 45 74 90 61 46 88	75	5.76E+06	3.39E+08
1-butanol	71-36-3	6.15	Medicine, Fruit	Fermented		4.90E-01	D 1		80	7.81E+03	1.59E+04
							D 2	4: 43 42 56 41	68	7.76E+04	1.58E+05
							D 5		73	1.90E+04	3.88E+04
Isobutanol	78-83-1	6.17	Wine, Solvent, Bitter	Ethereal, Winey			D 1	18: 43 41 42 33 39 74 40 72 56 57 38 59 44 53 73 60 51 37	97	1.29E+07	
							D 3	3: 42 41 43	73	2.60E+05	
							D 4	6: 43 57 41 42 56 39	68	1.23E+05	
							D 5	3: 39 42 41	65	5.14E+04	
Propanoic acid, anhydride	123-62-6	6.49					D 2	1: 57	69	2.88E+04	
							D 3	1: 57	76	8.26E+04	
							D 5	1: 57	65	3.15E+04	
4-methyl-3-penten-2-one	141-79-7	6.65	Sweet, Chemical	Pungent, Earthy, Vegetable, Acrylic		5.62E-02	D 3	5: 83 56 41 69 39	79	1.24E+05	2.21E+06
							D 4	5: 98 55 83 82 56	84	6.12E+04	1.09E+06
							D 5	3: 98 83 55	82	2.31E+04	4.11E+05
Decane	**124-18-5**	**6.66**	**Alkane**			**7.41E-01**	D 3		69	6.62E+04	8.93E+04
							E 1		82	3.45E+04	4.66E+04
Isoamyl alcohol	123-51-3	7.52	Whiskey, Malt, Burnt	Fusel oil, Alcoholic, Whiskey, Fruity, Banana		4.47E-02	D 1		69	2.43E+04	5.45E+05
							D 4	3: 55 70 53	66	1.40E+04	3.14E+05
Amyl alcohol	71-41-0	7.54	Balsamic	Fusel, Oil, Sweet, Balsam		4.68E-01	D 1		77	2.43E+04	5.20E+04
							D 4	3: 55 70 53	71	1.40E+04	3.00E+04
							D 5	2: 42 55	72	2.96E+04	6.34E+04
p-xylene	106-42-3	7.65				4.90E-01	D 3	2: 91 105	83	8.07E+04	1.65E+05

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
α-pinene	80-56-8	7.90	Pine, Turpentine	Herbal		6.92E-01	D 1		75	1.18E+04	1.70E+04
α-phellandrene	99-83-2	7.91	Turpentine, Mint, Spice	Terpenic			D 1		79	1.18E+04	
Camphene	79-92-5	10.21	Camphor	Woody			D 1		67	1.18E+04	
p-ethyltoluene	622-96-8	10.25					D 3	5: 120 105 91 155 136	76	4.89E+04	
2-ethyltoluene	611-14-3	10.61					D 3	4: 105 154 77 91	75	5.10E+04	
2,2,5-trimethylhexane	3522-94-9	10.67					D 3	7: 57 70 112 83 69 72 155	84	8.52E+05	
1-hexanol	111-27-3	10.73	Resin, Flower, Green	Herbal		4.37E-02	D 5	4: 69 56 41 42	66	7.45E+04	1.71E+06
Diacetone alcohol	123-42-2	10.79				8.91E-01	D 1		89	1.90E+05	2.14E+05
							D 4	10: 43 59 58 42 41 57 98 38 45 61	93	2.46E+06	2.76E+06
							D 5	7: 43 59 58 39 55 207 53	92	1.22E+06	1.37E+06
1,3,5-trimethylbenzene	108-67-8	11.02					D 3	7: 105 119 120 106 43 77 102	83	1.34E+05	
Piperidine	110-89-4	11.20		Animal		3.72E-01	D 3		79	1.29E+05	3.46E+05
2,4,5-trimethylbenzenamine	137-17-7	11.30					D 3	1: 120	73	1.13E+05	
Durene	95-93-2	11.36	Rancid, Sweet	Rancid		2.63E-02	D 1	2: 134 119	67	3.08E+04	1.17E+06
Isodurene	527-53-7	11.37					D 1	2: 134 119	68	1.76E+04	
							D 3	2: 119 134	70	4.14E+04	
1-ethyl-2,4-dimethylbenzene	874-41-9	11.38					D 3	2: 119 134	70	8.63E+04	
1,2,3,4-tetramethylbenzene	488-23-3	11.38				2.63E-02	D 1		78	2.05E+04	7.81E+05
p-cymene	99-87-6	11.38	Solvent, Gasoline, Citrus	Terpenic		2.14E-03	D 1		81	2.05E+04	9.61E+06
1,2,3,4-tetramethylbenzene	488-23-3	11.38				2.63E-02	D 3	2: 119 134	65	8.63E+04	3.28E+06
p-cymene	99-87-6	11.38	Solvent, Gasoline, Citrus	Terpenic		2.14E-03	D 3	2: 119 134	67	8.63E+04	4.04E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and <u>underlined</u> items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
N,N-dimethylbenzenamine	121-69-7	11.41					D 3	9: 120 105 121 103 79 91 97 77 122	82	2.62E+05	
3-phenyl propyl isobutyrate	103-58-2	11.41		Sweet, Fruity, Balsam			D 3	3: 118 117 141	69	1.09E+04	
3-phenyl propyl acetate	122-72-5	11.41		Sweet, Balsam, Storax, Spicy, Cinnamon			D 3	3: 118 117 141	67	1.09E+04	
2,4,6-trimethylbenzenamine	88-05-1	11.42					D 1		84	8.19E+04	
							D 3	1: 120	71	1.13E+05	
p-aminotoluene	106-49-0	11.53					D 3	4: 107 43 106 93	66	4.93E+04	
3,5-dimethylbenzenamine	108-69-0	12.00					D 3		78	1.88E+05	
2,4,6-trimethylpyridine	108-75-8	12.00					D 3	7: 120 121 77 56 66 57 122	73	3.46E+05	
Acetic acid	64-19-7	12.10	Sour	Acidic		1.45E-01	D 3	5: 43 60 42 41 61	99	4.73E+07	3.27E+08
							D 4		100	7.03E+07	4.87E+08
							D 5	6: 45 43 40 62 56 47	100	5.47E+07	3.78E+08
o-xylene	95-47-6	13.02	Geranium	Geranium		8.51E-01	D 3		73	6.49E+03	7.63E+03
Benzo[b]thiophene	95-15-8	13.39		Solvent, Rubbery, Earthy			D 1	1: 134	65	5.14E+04	
p-Hydroxyamphetamine acetate	96750-10-6	13.39					D 1		66	5.86E+04	
Nonanal	**124-19-6**	**13.64**	**Fat, Citrus, Green**	**Aldehydic**	**1.00E-03**	**2.24E-03**	D 1		69	1.28E+04	5.73E+06
							E 1		67	9.94E+03	4.44E+06
2-ethylhexanol	104-76-7	13.81	Rose, Green	Citrus		2.45E-01	D 1		88	2.79E+05	1.14E+06
							D 3	14: 42 98 70 112 39 58 113 84 69 72 54 68 99 51	98	4.65E+06	1.90E+07
Methyl vinyl ketone	78-94-4	13.90		Sweet			D 1	3: 41 70 55	69	6.55E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
Propanoic acid	79-09-4	13.90	Pungent, Rancid, Soy	Pungent, Acidic, Cheesy, Vinegar		3.55E-02	D 1	9: 74 44 55 38 56 57 46 37 58	67	1.92E+06	5.40E+07
							D 4	2: 73 74	94	2.04E+05	5.76E+06
							D 5		96	8.40E+04	2.37E+06
Propylene glycol	57-55-6	13.99					D 1	2: 45 73	66	4.09E+05	
							D 2		74	1.58E+05	
							D 4		96	5.72E+05	
							D 5	2: 45 55	93	2.58E+05	
Benzaldehyde	100-52-7	14.08	Almond, Burnt sugar	Fruity	3.00E-03	4.17E-02	D 1		97	7.61E+05	1.83E+07
							D 2	4: 77 105 106 51	88	3.14E+04	7.52E+05
							D 3	10: 107 76 74 52 39 49 108 73 37 64	98	4.88E+06	1.17E+08
							D 4	6: 105 77 106 51 50 52	95	2.19E+05	5.25E+06
							D 5		90	3.95E+04	9.47E+05
Indane	496-11-7	14.10					D 3	3: 118 117 141	67	1.09E+04	
Isobutyrophenone	**611-70-1**	**14.10**		**Green**			**D** 1	13: 105 77 51 78 106 74 75 49 38 50 76 52 39	76	1.35E+06	
							E 1	7: 37 105 119 121 118 93 62	80	4.77E+06	
Nonane	111-84-2	14.13	Alkane	Gasoline		1.26E+00	D 3		86	5.80E+04	4.61E+04
2-chloroacetophenone	**532-27-4**	**14.14**				**2.57E-02**	D 1	13: 105 77 51 78 106 74 75 49 38 50 76 52 39	87	1.35E+06	5.26E+07
							D 2		76	4.04E+04	1.57E+06
							D 3	10: 107 76 74 52 39 49 108 73 37 64	76	4.88E+06	1.90E+08
							D 4	6: 105 77 106 51 50 52	74	2.19E+05	8.52E+06
							D 5		69	3.95E+04	1.54E+06
							E 1	7: 37 105 119 121 118 93 62	92	3.56E+05	1.38E+07
Undecane	1120-21-4	14.14	Alkane			1.17E+00	D 3	5: 127 53 55 39 72	78	9.14E+05	7.78E+05

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
2,2-dimethylbutane	75-83-2	14.15					D 3	3: 41 71 56	84	2.69E+05	
Dodecane	**112-40-3**	**14.15**	**Alkane**	**Alkane**		**2.04E+00**	E 1		95	2.59E+05	1.27E+05
Tridecane	629-50-5	14.17	Alkane	Alkane		2.14E+00	D 1	8: 41 56 57 86 85 99 112 70	74	3.03E+05	1.42E+05
							D 3	8: 85 127 57 55 82 70 128 126	76	6.23E+05	2.92E+05
Octyl acetate	112-14-1	14.20		Green, Earthy, Mushroom, Herbal, Waxy		3.98E-03	D 1	4: 56 57 55 43	76	7.44E+04	1.87E+07
N-Nitrosodimethylamine	62-75-9	14.66					D 5	3: 74 43 57	70	2.72E+05	
Ethyl lactate	97-64-3	14.90	Fruit	Sharp, Tart, Fruity, Buttery, Butterscotch		1.62E+00	D 5	2: 45 55	68	4.23E+05	2.61E+05
2-Hydroxyethylhydrazine	109-84-2	14.91					D 4		65	5.72E+05	
							D 5		67	5.15E+04	
Ethyl octanoate	**106-32-1**	**15.23**	**Fruit, Fat**	**Fruity, Wine, Waxy, Sweet, Apricot, Banana, Brandy, Pear**		**5.75E-04**	E 1	9: 101 43 73 102 88 61 60 129 168	87	9.77E+04	9.77E+04
tetrahydro-2-methyl-2-furanol	7326-46-7	15.59					D 3	2: 71 69	77	6.97E+04	
							D 4		76	1.27E+04	
1-methyl-1H-pyrrole	96-54-8	15.72		Smoky, Woody, Herbal			D 2	1: 81	69	2.94E+04	
2-ethoxyethanol	110-80-5	15.79				1.23E+00	D 1	3: 59 60 37	74	1.19E+05	9.65E+04
Hexestrol	84-16-2	15.85					D 1		73	8.19E+04	
Methyl benzoate	**93-58-3**	**16.30**	**Prune, Lettuce, Herb, Sweet**	**Phenolic**		**1.07E-01**	D 1	11: 105 77 136 76 137 106 39 49 75 74 91	99	1.81E+06	1.69E+07

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
							E 1	10: 105 77 92 49 52 152 64 181 127 141	100	1.35E+08	1.26E+09
Cumene	98-82-8	16.49				2.40E-02	D 3	5: 105 135 120 77 78	77	2.84E+05	1.18E+07
Acetophenone	98-86-2	16.49	Musty, Flower, Almond	Floral	6.50E-02	3.63E-01	D 3	5: 105 135 120 77 78	93	2.84E+05	7.81E+05
3-ethyltoluene	620-14-4	16.50					D 3	4: 78 105 120 106	78	1.52E+05	
2,2,4-trimethylpentane	540-84-1	16.53					D 1	4: 56 57 55 43	66	8.44E+04	
							D 3	3: 41 57 56	88	2.57E+05	
2-ethyl-5-methylpyrazine	13360-64-0	16.81	Fruit, Sweet	Coffee bean, Nutty			D 3	3: 121 122 81	73	3.39E+04	
γ-hexalactone	695-06-7	17.20	Coumarin, Sweet	Tonka			D 3	4: 56 85 69 51	68	2.89E+05	
2-ethyl-3,5-dimethylpyridine	1123-96-2	17.90					D 1		91	5.86E+04	
							D 3	4: 107 135 134 70	86	1.49E+05	
α-α-Dimethylbenzenemethanol	617-94-7	18.05		Mild, Green, Sweet, Earthy			D 3	6: 122 105 78 77 136 102	89	1.71E+05	
p-methoxyphenylacetone	122-84-9	18.07		Sweet, Fruity, Spicy, Anisic, Balsam			D 3		68	9.60E+04	
3-methylhexane	589-34-4	18.33					D 1		70	4.60E+03	
							D 3	7: 43 70 41 56 39 42 100	97	5.33E+05	
Tetradecane	629-59-4	18.34	Alkane	Mild, Waxy			D 1	5: 198 140 154 82 100	98	3.83E+06	
1-undecanol	**112-42-5**	**18.37**	**Mandarin**	**Waxy**		**6.76E-02**	E 1	4: 111 83 97 106	74	2.87E+04	4.24E+05
Nitrocyclohexane	1122-60-7	19.50					D 3	5: 83 56 41 69 39	74	2.15E+05	
β-caryophyllene	87-44-5	19.68	Wood, Spice	Spice	6.40E-02		D 1		66	1.51E+04	2.36E+05
							D 2		69	1.18E+04	1.84E+05
							D 3		85	7.37E+04	1.15E+06

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 10 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
Pentadecane	629-62-9	20.28	Alkane	Waxy			D 1	8: 41 56 57 86 85 99 112 70	86	1.74E+05	
Butanoic acid, butyl ester	109-21-7	20.97		Fruity, Banana, Pineapple, Sweet			D 1		76	3.03E+04	
Longifolene	475-20-7	21.28		Wood			D 3		74	7.37E+04	
Toluene-2,4-diamine	95-80-7	23.91					D 3	3: 121 122 81	72	3.39E+04	
2,3,6-trimethylpyridine	1462-84-6	23.96					D 3		74	1.06E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Cocaine.

SI Table 11. Summary of VOCs emitted from all illicit heroin samples and Sigma Pseudo™ Narcotic Scent Heroin formulation over 1 hour at room temperature. Sigma Pseudo™ Narcotic Scent Heroin formulation is indicated by underlined and **bolded** fonts.

SI Table 11 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
Ethylene oxide	**75-21-8**	**1.06**				**8.51E+02**	F 1	3: 44 45 46	66	3.54E+06	4.16E+03
							G 1	4: 44 45 46 43	68	1.75E+06	2.06E+03
2-nitropropane	79-46-9	1.12				7.24E+00	F 2	3: 43 41 58	74	1.30E+04	1.80E+03
Methyl chloride	74-87-3	1.15					F 1	2: 50 52	73	1.00E+04	
Isobutanol	78-83-1	1.19	Wine, Solvent, Bitter	Ethereal, Winey			F 1		70	4.81E+04	
							F 2	6: 42 57 43 41 56 39	68	8.76E+04	
Hexane	110-54-3	1.19	Alkane			2.19E+01	F 1	6: 43 41 57 42 56 39	82	7.74E+04	3.54E+03
							F 2	6: 42 57 43 41 56 39	82	8.76E+04	4.00E+03
Isobutane	75-28-5	1.23				1.00E+01	F 1	10: 43 42 41 57 72 39 55 56 38 58	83	8.96E+05	8.96E+04
							F 2	13: 43 42 41 72 39 57 56 63 53 38 73 58 37	83	1.18E+06	1.18E+05
Isobutyraldehyde	78-84-2	1.23	Pungent, Malt, Green	Spicy		4.07E-02	F 1	10: 43 42 41 57 72 39 55 56 38 58	78	8.96E+05	2.20E+07
							F 2	13: 43 42 41 72 39 57 56 63 53 38 73 58 37	77	1.18E+06	2.89E+07
4-methyldecane	2847-72-5	1.39					F 1	4: 71 57 41 72	67	4.33E+05	
							F 2	9: 43 42 41 39 55 85 53 38 69	66	4.19E+05	
2-methylpentane	107-83-5	1.39					F 1	4: 71 57 41 72	97	4.33E+05	
							F 2	9: 43 42 41 39 55 85 53 38 69	97	4.19E+05	
Ethylenimine	151-56-4	1.40					F 2	9: 43 42 41 39 55 85 53 38 69	86	3.48E+05	
2,3-dimethylbutane	79-29-8	1.40					F 2	9: 43 42 41 39 55 85 53 38 69	81	3.48E+05	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Heroin.

SI Table 11 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
3,4,5-trimethyl-1-hexene	56728-10-0	1.40					F 1		68	2.72E+05	
							F 2	8: 71 43 57 56 70 51 39 86	67	3.94E+05	
3-methylhexane	589-34-4	1.40					F 2	8: 71 43 57 56 70 51 39 86	75	2.78E+05	
1-butanol	**71-36-3**	**1.42**	**Medicine, Fruit**	**Fermented**		**4.90E-01**	F 1	6: 43 41 57 42 56 39	66	7.74E+04	1.58E+05
							F 2		81	1.12E+04	2.29E+04
							G 1	4: 39 41 69 43	72	6.39E+04	1.30E+05
3-methylpentane	96-14-0	1.45					F 1	3: 71 56 57	87	5.52E+04	
							F 2		88	2.45E+04	
2-methylaziridine	75-55-8	1.49					F 1	3: 71 56 57	79	5.52E+04	
							F 2	2: 41 56	80	3.37E+04	
Isocyanatomethane	624-83-9	1.52					F 1		77	1.32E+04	
Tolycaine	3686-58-6	1.52					F 1	1: 86	67	8.96E+02	
Propene	115-07-1	1.65				5.25E+01	F 2	3: 42 39 41	73	3.41E+04	6.50E+02
Butane	106-97-8	1.66				2.04E+02	F 1	4: 58 43 42 38	74	1.45E+05	7.10E+02
							F 2		79	2.36E+05	1.15E+03
Acetone	67-64-1	1.66		Solvent		1.45E+01	F 1	4: 58 43 42 38	92	1.45E+05	1.00E+04
							F 2	5: 43 58 39 37 38	97	3.14E+05	2.18E+04
Hydrazine	302-01-2	1.97				3.00E+00	F 1	1: 33	78	1.19E+03	3.97E+02
Cyclohexane	**110-82-7**	**1.98**				**2.19E+01**	G 1	9: 39 84 56 42 55 69 85 50 54	96	2.71E+05	1.24E+04
Ethylacetate	141-78-6	2.32	Pineapple	Ethereal, Fruity, Sweet, Weedy, Green		2.63E+00	F 2		96	2.41E+05	9.17E+04
Propylene glycol	57-55-6	2.33					F 1	2: 43 45	69	5.16E+04	
							F 2	3: 45 61 44	65	8.74E+04	
Isopropyl alcohol	67-63-0	2.33		Alcohol, Musty, Woody		1.02E+01	F 1	2: 43 45	69	2.14E+04	2.09E+03
Ethanol	64-17-5	2.33	Sweet	Alcoholic		2.88E+01	F 2	3: 45 61 44	68	6.90E+04	2.39E+03
Acetic anhydride	**108-24-7**	**3.66**		**Sharp, Vinegar**		**5.89E-01**	F 1	2: 43 42	76	6.24E+03	1.06E+04
							F 2	4: 43 37 42 38	71	1.43E+05	2.43E+05
							G 1	1: 43	69	3.64E+04	6.18E+04
nitrocyclohexane	**1122-60-7**	**10.29**					G 1	3: 83 55 41	74	2.39E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Heroin.

SI Table 11 continued

Compound	CAS	RT (min)	Published Descriptors: Flavornet[1]	Published Descriptors: TGSC[2]	Published ODT (ppm): LRI & Odour[3]	Published ODT (ppm): Devos, *et al.*[4]	Code	Models	Net % Match	PAC	OAV
m-cymene	**535-77-3**	**11.33**					G 1		93	4.08E+04	
1-(3-methylphenyl)-ethanone	**585-74-0**	**11.34**					G 1		86	2.84E+04	
tert-butyl-benzene	**98-06-6**	**11.34**					G 1		88	2.84E+04	
1,2,3,4-tetramethylbenzene	**488-23-3**	**11.35**				**2.63E-02**	F 1	3: 120 119 134	66	2.94E+04	1.12E+06
p-cymene	**99-87-6**	**11.35**	**Solvent, Gasoline, Citrus**	**Terpenic**		**2.14E-03**	F 1	3: 120 119 134	65	2.94E+04	1.37E+07
							G 1		91	4.08E+04	1.91E+07
1,2,3,4-tetramethylbenzene	**488-23-3**	**11.35**				**2.63E-02**	G 1		86	4.08E+04	1.55E+06
Isodurene	527-53-7	11.37					F 1	3: 120 119 134	69	2.94E+04	
Acetic acid	**64-19-7**	**12.09**	**Sour**	**Acidic**		**1.45E-01**	F 1	5: 43 60 41 59 47	97	5.74E+07	3.97E+08
							F 2		99	2.62E+05	1.81E+06
							G 1	5: 45 43 60 46 105	100	5.84E+07	4.04E+08
Nitrogen dioxide	**10102-44-0**	**12.29**				**1.86E-01**	G 1	1: 46	76	9.21E+02	4.95E+03
Furfural	98-01-1	12.71	Bread, Almond, Sweet	Sweet, Woody, Almond, Baked bread		7.76E-01	F 2		93	3.22E+04	4.15E+04
Fenbendazole	43210-67-9	12.98					F 1	3: 267 269 268	66	5.95E+04	
Propanoic acid	79-09-4	13.91	Pungent, Rancid, Soy	Pungent, Acidic, Cheesy, Vinegar		3.55E-02	F 1		94	9.03E+04	2.54E+06
Propanoic acid, anhydride	**123-62-6**	**13.91**					F 2	5: 57 209 193 82 69	68	3.17E+03	
							G 1	1: 57	66	4.74E+03	
Benzaldehyde	**100-52-7**	**14.10**	**Almond, Burnt sugar**	**Fruity**	**3.00E-03**	**4.17E-02**	G 1	2: 105 77	76	5.40E+04	1.30E+06
2-chloroacetophenone	**532-27-4**	**14.10**				**2.57E-02**	G 1	2: 105 77	77	5.40E+04	2.10E+06
Isobutyrophenone	**611-70-1**	**14.10**		**Green**			G 1	2: 105 77	66	3.06E+04	
Ethyl cyclohexane	**1678-91-7**	**15.20**					G 1	1: 83	70	7.33E+04	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Heroin.

SI Table 11 continued

			Published Descriptors		Published ODT (ppm)						
Compound	**CAS**	**RT (min)**	**Flavornet[1]**	**TGSC[2]**	**LRI & Odour[3]**	**Devos, *et al.*[4]**	**Code**	**Models**	**Net % Match**	**PAC**	**OAV**
Butyric acid	107-92-6	15.53	Rancid, Cheese, Sweat	Sharp, Acetic, Cheese, Butter, Fruit		3.89E-03	F 1	3: 60 42 37	95	4.20E+05	1.08E+08
Pentanoic acid	109-52-4	15.53	Sweat	Sickening, Putrid, Acidic, Sweaty, Rancid		4.79E-03	F 1	5: 60 45 73 43 39	89	3.45E+05	7.22E+07
2,2-dimethylbutane	75-83-2	15.87					F 1		82	1.06E+04	
Methyl benzoate	**93-58-3**	**16.26**	**Prune, Lettuce, Herb, Sweet**	**Phenolic**		**1.07E-01**	G 1		97	1.74E+05	1.63E+06
Toluene	108-88-3	19.16	Paint	Sweet		1.55E+00	F 2		80	2.84E+04	1.84E+04
Dimethylsulfone	67-71-0	20.11	Sulfur, Burnt	Sulfurous, Burnt			F 2	2: 79 62	96	1.94E+05	
Methyl formate	**107-31-3**	**22.87**		**Fruity, Plum**		**9.33E+01**	G 1	1: 60	73	1.83E+03	1.96E+01
Diethyl Phthalate	84-66-2	27.46					F 1		69	9.71E+03	

If two ODTs are available, ODT from Devos, *et al.* is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Table 3. Models = significant ions used for identification/semi-quantitation, # before colon is number of significant ions, #'s after colon are *m/z*. Net % match as calculated using AMDIS and target specialty mass spectral libraries. PAC = Peak Area Counts, and refers to relative abundance as given by the mass spectral detector. OAV = Odor Activity Value, and is calculated as ratio of PAC: OAV. **Bolded** and underlined items highlight the compounds found in Pseudo Scent Heroin.

References

1 Acree, T. E. & Arn, H. Flavornet and human odor space. http://flavornet.org/flavornet.html (2004). Accessed September 8, 2014

2 The Good Scents Company Information System. http://www.thegoodscentscompany.com/index.html# (1994). Accessed August 8, 2014.

3 Mottram, R. LRI & Odour Database. www.odour.org.uk/index.html (2006). Accessed August 1, 2014.

4 M. Devos, F. P., J. Rouault, P. Laffort, L.J. Van Gemert. Standardized Human Olfactory Thresholds. (IRL Press at Oxford Press, 1990).

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