Data Article

Odor impact of volatiles emitted from marijuana, cocaine, heroin and their surrogate scents

Somchai Rice\textsuperscript{a,b}, Jacek A. Koziel\textsuperscript{a,b,*}

\textsuperscript{a} Department of Agricultural and Biosystems Engineering, Iowa State University, Ames, IA 50011, USA
\textsuperscript{b} Interdepartmental Toxicology Graduate Program, Iowa State University, Ames, IA 50011, USA

\textbf{Abstract}

Volatile compounds emitted into headspace from illicit street drugs have been identified, but until now odor impact of these compounds have not been reported. Data in support of identification of these compounds and their odor impact to human nose are presented. In addition, data is reported on odor detection thresholds for canines highlighting differences with human ODTs and needs to address gaps in knowledge. New data presented here include: (1) compound identification, (2) gas chromatography (GC) column retention times, (3) mass spectral data, (4) odor descriptors from 2 databases, (5) human odor detection thresholds from 2 databases, (6) calculated odor activity values, and (7) subsequent ranking of compounds by concentration and ranking of compounds by odor impact (reported as calculated odor activity values). For further interpretation and discussion, see Rice and Koziel\textsuperscript{[1]} and Rice\textsuperscript{[2]}.

© 2015 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

\textbf{Specifications table}

\begin{tabular}{|c|c|}
\hline
Subject area & Chemistry \\
\hline
More specific subject area & Forensics, Analytical Chemistry, Olfactometry \\
Type of data & Table \\
\hline
\end{tabular}

DOI of original article: http://dx.doi.org/10.1016/j.forsciint.2015.08.027
* Corresponding author.
E-mail address: koziel@iastate.edu (J.A. Koziel).

http://dx.doi.org/10.1016/j.dib.2015.09.053
2352-3409© 2015 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).
How data was acquired

Multidimensional gas chromatography (Agilent 6890), mass spectroscopy (Agilent 5973), olfactometry (MOCON, Round Rock, TX).

Data format

Analyzed mass spec using Automatic Mass Spectral Deconvolution and Identification System (AMDIS) (NIST, Gaithersburg, MD).

Experimental factors

Volatile emissions from marijuana, cocaine, and heroin samples were collected on Carboxen/polydimethylsiloxane (PDMS) solid-phase microextraction (SPME) fiber at room temperature, static, for 1 h.

Experimental features

SPME fibers were thermally desorbed in a multidimensional gas chromatography-mass spectrometry-olfactometry (MDGC-MS-O) instrument, allowing for simultaneous chemical and sensory analysis. Surrogate scents for each drug were also analyzed as previously stated, and aromas were compared using calculated odor activity values (OAVs).

Data source location

Department of Agricultural and Biosystems Engineering at Iowa State University, Ames, IA 50011.

Data accessibility

Data is with this article.

Value of the data

- This data is the most comprehensive summary of volatiles emitted from real and surrogate scents of marijuana (221, 78), cocaine (153, 15), and heroin (41, 19), respectively, to date.
- This data includes organoleptic percepts from 2 known databases, odor detection thresholds from 2 benchmark databases, significant ions from mass spectral data, and calculated odor activity values (OAVs, if available) for each compound.
- This data shows rank of drug volatiles by concentration in relation to the rank by odor impact (as calculated OAV).
- Odor activity value data can open up new ways of forensic drug analysis.
- Data from previous research on canine odor detection thresholds (ODTs) is reported for further insight, highlighting differences with human ODTs and needs to address gaps in knowledge.

1. Data

1.1. CAS Registry Number

A CAS Registry Number is a unique numeric identifier that corresponds to only one substance. The CAS has no chemical significance, but can be used as a link to more information about a specific chemical substance [3]. CAS number is useful to identify a compound that has multiple synonyms. CAS numbers were used in all data tables in this report.

1.2. Odor Detection Threshold (ODTs)

Published ODT values are not fixed numbers, but are set to represent the lowest concentration that 50% of the population can detect [4]. For the purposes of calculating odor activity values, standardized human ODTs from Devos et al. [5] were used when available. The compilation from Devos et al. contained a total of 2075 ODT values in air for 641 chemical compounds, gathered from 372 references. ODTs were weighted and averaged [5]. If ODT for a compound was not given in Devos et al., the LRI Database [6] was used. LRI database contains 1500+ records on ODT and odor percepts [6]. ODTs for canines were compiled from previous literature. See Rice and Koziel [1] for full discussion on human and canine ODTs. ODTs were used in reporting data in Tables 1–5.

1.3. Column retention time in chromatography

Column retention time (RT, min) is the time between sample introduction via thermal desorption in the gas chromatography (GC) inlet and the analyte peak reaching the mass spectrometer and/or
sniff port at the end of the analytical column. It was not appropriate to use retention indexes (Kovats RI) for identification because: (1) the non-polar and polar columns were connected in series when analyzing in multidimensional GC; (2) use of indices of medium polarity column could lead to large errors for compounds that are affected by one of the columns more than the other. Known retention times of standards previously analyzed on this system were used for compound identification, and indicated by + symbol in Tables 3–5. RTs are also reported in Tables 3–5.

1.4. Aroma descriptors

Aroma descriptors were compiled from Flavornet and The Good Scents Company. Flavornet has aroma descriptors from 738 compounds, compiled from studies using GC-olfactometry [7]. The Good Scents Company is dedicated to providing organoleptic information to the flavor, food and fragrance industry [8]. Aroma descriptors from these 2 databases were used in reporting data in Tables 3–5.

1.5. Sample code

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 (Sample Code A1–A3); (2) 1 g marijuana packaged in a plastic zip-top sandwich bag (Sample Code A4–A5); (3) 1 g old, desiccated marijuana with no packaging (Sample Code A6–A7); (4) plastic zip-top sandwich bag with 1 g marijuana removed (Sample Code B1–B4); (5) 1 g crack cocaine packaged as tear drops (Sample Code D1); (6) 1 g cocaine adulterated with Levamisole (Sample Code D2); (7) 1 kg evidence pack containing cocaine (Sample Code D3); (8) 1 g cocaine in an opened plastic bag (Sample Code D4–D5); (9) 1 g heroin seized in 1997 (Sample Code F1); (10) 1 g heroin seized in 2010 (Sample Code F2). Sigma Pseudo™ Narcotic Scent Marijuana formulation (Fluka, P7309) (Sample Code C1–C3), Sigma Pseudo™ Narcotic Scent Cocaine formulation (Fluka, P2423) (Sample Code E1), and Sigma Pseudo™ Narcotic Scent Heroin formulation (Fluka, P2548) (Sample Code G1) were purchased from Sigma-Aldrich (St. Louis, MO). These sample codes were used in reporting data in Tables 3–5.

1.6. Target mass spec libraries, models, and net % match, peak area counts

AMDIS (NIST, Gaithersburg, MD) software was used for identification of unknown compounds. Six specialty mass spectral libraries were used for compound identification: NISTEPA (1086 compounds in the EPA’s ‘list of lists’), NISTDRUG (739 compounds in the Canadian AAFS Toxicology Section MS Database Committee and the Association of Official Racing Chemists libraries), NISTFF (991 compounds in the Philip Morris Flavor and fragrance collection), NISTTOX (1213 compounds represented in Finnigan Corporation’s Toxicology library), NISTFDA (415 compounds in an FDA collection of mass spectra), and NISTCW (62 compounds relevant to detection of chemical weapons).

A model is the mass-to-charge ratio (m/z) of a deconvoluted peak, and are listed in order of highest to lowest relative abundance. For example, under a ‘Models’ column heading, 2: 58 88 signifies 2 models with m/z 58 and 88 were used for identification.

Net % Match is the final match quality value (100 = perfect match) between the deconvoluted component and the target library spectra. The minimum match value was set at 65 for all analysis of this data.

Peak area counts (PAC) refers to the relative abundance of the analyte, or the area under the chromatographic peak. The mass detector was assumed to have equal response factors for each compound, for the purposes of calculating OAV.

These parameters were used in reporting data in Tables 3–5.

1.7. Odor activity values (OAV)

OAV is defined as the unit less ratio of concentration of a compound in gas phase to the odor detection threshold. For illustrative purposes, the PAC was used for the concentration value of each compound. See Rice and Koziel [1] and Rice [2] for further discussion on OAV. This ratio was used to calculate the OAVs reported in Tables 3–5.
1.8. Ranking definitions

Compounds from each drug were ranked by concentration (highest concentration = ranked 1) and then by calculated OAV (highest odor impact = ranked 1). In most cases, there was no apparent correlation between chemical concentration and odor impact, i.e., rank 1 by concentration did not usually rank as 1 by OAV. This ranking and sorting was used to report data in Tables 6–8.

2. Experimental design, materials and methods

2.1. Surrogate scent formulations

Sigma Pseudo™ Narcotic Scent Marijuana formulation composition is listed as pyrogenic colloidal silica (1%), cellulose (98.5%), butane-2,3-diol (0.4%), and p-mentha-1,4-diene (0.1%). Sigma Pseudo™ Narcotic Scent Cocaine formulation composition is listed as cellulose (98.9%), pyrogenic colloidal silica (1%), and methyl benzoate (0.1%). Sigma Pseudo™ Narcotic Scent Heroin formulation composition is listed as cellulose (74.1%), o-acetylsalicylic acid (25.2%), acetic acid (0.3%), and pyrogenic colloidal silica (0.3%).

2.2. Methodology

Carboxen/PDMS, 85 μm Stable-flex, 24 gauge SPME fibers were used (Sigma-Aldrich, St. Louis, MO, USA). Briefly, experimental conditions were as follows: drugs were placed in separate, pre-cleaned and oven-baked 16 ounce mason jars with modified lids. The Carboxen/PDMS SPME fibers were exposed to the headspace and volatiles were passively extracted; equilibration time was the same as extraction time (1 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 were stored as described above in a 4 °C refrigerator pending placement into the heated injection port of the MDGC-MS-O for thermal desorption and analysis.

MDGC-MS-O analysis was performed on an Agilent 6890 GC, with a restrictor guard column, non-polar capillary column (BP-5, 56 m × 530 μm inner diameter × 1.00 μm thickness, SGE, Austin, TX, USA) and polar capillary column (BP-20, 25 m × 530 μm inner diameter × 1.00 μm thickness, SGE, Austin, TX, USA) connected in series. Outflow from analytical column was held at 70 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 min in splitless mode at 270 °C under flow of helium carrier gas (99.995% purity). Analysis of the same fiber immediately after sample injection, revealed no carry over, with all compounds desorbed in the initial analysis. The oven temperature was programmed as follows: 40 °C for 3.00 min, then increased to 220 °C at a rate of 700 °C per min, and held for 11.29 min (40 min 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 70 eV, with acquisition range m/z 33–280.

The instrument was tuned daily and analysis of column blanks 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 of each sampling run did not demonstrate contaminating compounds. VOCs were identified tentatively using the Automatic Mass Spectral Deconvolution and Identification System (AMDIS) (National Institute of Standards and Technology, Gaithersburg, MD) and six specialty mass spectral libraries provided derived from the NIST05/EPA/NIH mass spectral database. Known retention times of standards previously analyzed on this system were used for identification. Chemical standards available in house were analyzed to match retention times and mass spectra of unknown compounds. Select reference standards were used for identification, purchased from Sigma-Aldrich (St. Louis, MO, USA). These standards are indicated with ‘+’ in Tables 3–5. Each sample (as outlined in Section 1.5) was collected on a single SPME fiber, each fiber sample was analyzed by one panelist. The same panelist analyzed all samples with volatiles from each drug and surrogate scent formulation.
Table 1
Comparison of odor detection thresholds and odor activity values between canines (based on Passe and Walker [9]) and humans (based on Devos et al. [5]).

| Source reference in [9] | Methods | Compound | CAS     | Canine ODT [9] (ppm) | Human ODT [5] (ppm) | ODT<sub>C</sub>:ODT<sub>H</sub> | Canine OAV of 1 ppm | Human OAV of 1 ppm | OAV<sub>C</sub>:OAV<sub>H</sub> |
|-------------------------|---------|----------|---------|----------------------|---------------------|-----------------------------|----------------------|----------------------|----------------------|
| Neuhaus [10]            | Dogs chose from 3 odor ports. Pushing a box behind the correct port uncovered sugar for reward. | Acetic acid | 64-19-7 | 4.99E-11 | 1.45E-01 | 3.44E-10 | 2.00E+10 | 6.90E+00 | 2.90E+09 |
|                         |         | Propanoic acid | 79-09-4 | 3.09E-11 | 3.55E-02 | 8.70E-10 | 3.24E+10 | 2.82E+01 | 1.15E+09 |
|                         | Butyric acid | 107-92-6 | 1.46E-12 | 3.89E-03 | 3.76E-10 | 6.84E+11 | 2.57E+02 | 2.66E+09 |         |
|                         |         | Pentanoic acid | 109-52-4 | 5.36E-12 | 4.79E-03 | 1.12E-09 | 1.87E+11 | 2.09E+02 | 8.94E+08 |
|                         |         | Hexanoic acid | 142-62-1 | 7.67E-12 | 1.26E-02 | 6.09E-10 | 1.30E+11 | 7.94E+01 | 1.64E+09 |
|                         |         | Octanoic acid | 124-07-2 | 1.20E-11 | 3.98E-03 | 3.01E-09 | 8.34E+10 | 2.51E+02 | 3.32E+08 |
| Ashton, Eayrs and Moulton [11] | Crucibles containing odorous solutions was placed on the floor. Dog alerted by sitting when odor was present. | Formic acid | 64-18-6 | 1.30E+03 | 2.82E+01 | 4.60E+01 | 7.71E-04 | 3.55E-02 | 2.17E-02 |
|                         |         | Acetic acid | 64-19-7 | 1.73E+02 | 1.45E-01 | 1.19E+03 | 5.77E-03 | 6.90E+00 | 8.37E-04 |
|                         |         | Propanoic acid | 79-09-4 | 1.78E+01 | 3.55E-02 | 5.01E+02 | 5.63E-02 | 2.82E+01 | 2.00E-03 |
|                         | Butyric acid | 107-92-6 | 3.67E+00 | 3.89E-03 | 9.44E+02 | 2.72E-01 | 2.57E+02 | 1.06E-03 |         |
|                         |         | Pentanoic acid | 109-52-4 | 5.24E+01 | 4.79E-03 | 1.09E+04 | 1.91E-02 | 2.09E+02 | 9.14E-05 |
|                         |         | Hexanoic acid | 142-62-1 | 3.20E+01 | 1.26E-02 | 2.54E+03 | 3.13E-02 | 7.94E+01 | 3.94E-04 |
|                         |         | Heptanoic acid | 111-14-8 | 1.76E+01 | 2.75E-02 | 6.39E+02 | 5.69E-02 | 3.64E+01 | 1.57E-03 |
|                         |         | Octanoic acid | 124-07-2 | 8.11E+00 | 3.98E-03 | 2.04E+03 | 1.23E-01 | 2.51E+02 | 4.91E-04 |
| Moulton, Ashton, and Eayrs [12] | Crucibles containing odorous solutions was placed on the floor. Dog alerted by sitting when odor was present. | Formic acid | 64-18-6 | 1.96E-02 | 2.82E+01 | 6.96E-04 | 5.09E+01 | 3.55E-02 | 1.44E+03 |
|                         |         | Acetic acid | 64-19-7 | 5.73E-04 | 1.45E-01 | 3.95E-03 | 1.74E+03 | 6.90E+00 | 2.53E+02 |
|                         |         | Propanoic acid | 79-09-4 | 1.23E-05 | 3.55E-02 | 3.46E-04 | 8.13E+04 | 2.82E+01 | 2.89E+03 |
|                         | Butyric acid | 107-92-6 | 4.95E-07 | 3.89E-03 | 1.27E-04 | 2.02E+06 | 2.57E+02 | 7.85E+03 |         |
|                         |         | Pentanoic acid | 109-52-4 | 1.55E-05 | 4.79E-03 | 3.23E-03 | 6.47E+04 | 2.09E+02 | 3.10E+02 |
|                         |         | Hexanoic acid | 142-62-1 | 3.13E-06 | 1.26E-02 | 2.48E-04 | 3.20E+05 | 7.94E+01 | 4.03E+03 |
|                         |         | Heptanoic acid | 111-14-8 | 5.55E-07 | 2.75E-02 | 2.02E-05 | 1.80E+06 | 3.64E+01 | 4.95E+04 |
|                         |         | Octanoic acid | 124-07-2 | 1.12E-07 | 3.98E-03 | 2.81E-05 | 8.93E+06 | 2.51E+02 | 3.56E+04 |
|                         |         | Isobutyric acid | 79-31-2 | 5.56E-07 | 1.95E-02 | 2.85E-05 | 1.80E+06 | 5.13E+01 | 3.51E+04 |
| Source reference in [9] | Methods | Compound | CAS [9] (ppm) | Canine ODT [5] (ppm) | Human ODT [5] (ppm) | ODT<sub>C</sub>: ODT<sub>H</sub> | Canine OAV of 1 ppm | Human OAV of 1 ppm | OAV<sub>C</sub>: OAV<sub>H</sub> |
|-------------------------|---------|----------|--------------|---------------------|---------------------|------------------|----------------|----------------|------------------|
| Moulton and Marshal [13] | Trial was initiated by manipulating a treadle, dogs chose from 3 odor ports. Alert was placing nose in correct odorant for 5 seconds. | α-ionone | 127-41-3 | 4.02E-13 | 5.75E-05 | 6.99E-09 | 2.49E +12 | 1.74E +04 | 1.43E +08 |
| Marshall, Blumer and Moulton [14] | Same test apparatus as Moulton and Marshal (1976). 1 sample port, alert was keeping nose in port for 5 sec. | Pentanoic acid | 109-52-4 | 1.51E-07 | 4.79E-03 | 3.15E-05 | 6.62E +06 | 2.09E +02 | 3.17E +04 |
| Krestel, Passe, Smith and Jonsson [15] | Conditioned suppression using odor ports. | Amyl acetate | 628-63-7 | 1.93E-07 | 3.09E-02 | 6.23E-06 | 5.19E +06 | 3.24E +01 | 1.60E +05 |

REF = reference; ODT = odor detection threshold; OAV = odor activity value; ODT<sub>C</sub> = canine odor detection threshold; ODT<sub>H</sub> = human odor detection threshold; OAV<sub>C</sub> = odor activity value for canines; OAV<sub>H</sub> = odor activity value for humans. All gas phase calculations assumed 1 atm at 25 °C.
Table 2
Comparison of ODT and OAV in canines vs. humans in two recent field studies.

| REF | Method | Mixture ratio | Compound | CAS | Conc. tested (ppm) | % of canines alerted | Canine ODT (ppm) | Human ODT (ppm) | ODT\text{C}:ODT\text{H} | Canine OAV of 1 ppm | Human OAV of 1 ppm | OAV\text{C}:OAV\text{H} |
|-----|--------|---------------|----------|-----|--------------------|---------------------|------------------|----------------|-------------------|-----------------|-----------------|------------------|
| Lorenzo, Wan, Harper, Hsu, Chow, Rose, Furton [16] | Scent solution was spiked onto filter paper, placed in a metal box with holes drilled on top. | | Insosafrole | 120-58-1 | 6.76E+02 | 0 | 6.27E+02 | 1.60E-03 | 1.95E+01 | 2.09E+02 | 7.35E-06 | | |
| | | | Phorone | 504-20-1 | 6.27E+02 | 4 | 5.13E-02 | 1.36E+05 | 1.53E-03 | | | |
| | | | Camphor | 76-22-2 | 6.43E+02 | 0 | 6.27E+02 | 9.55E-03 | 1.60E-03 | 9.60E+00 | | |
| | | | Piperonal | 120-57-0 | 6.52E+02 | 17 | 4.79E-03 | 2.31E+04 | 1.04E-03 | 2.40E+01 | 4.33E-05 | |
| | | | Benzaldehyde | 94-59-7 | 6.61E+02 | 0 | 5.13E-02 | 3.60E+00 | 1.95E-03 | | | |
| | | | Acetic acid | 120-57-0 | 1.71E+03 | 0 | 1.45E-01 | 4.17E-04 | 2.12E-06 | 1.76E-06 | | |
| | | | 1-phenyl-2-propanol | 100-86-7 | 6.35E+02 | 9 | 6.35E-02 | 7.35E-06 | | | | |
| | | | Acetophenone | 98-86-2 | 8.37E+02 | 0 | 3.63E-01 | 2.31E+00 | 2.40E+01 | 4.33E-05 | | |
| | 1:1 | MD-P2P | Insosafrole | 4676-39-5 | 5.49E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | Piperonal | 120-57-0 | 6.52E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | 3:1 | MD-P2P | Insosafrole | 4676-39-5 | 6.52E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | Piperonal | 120-57-0 | 6.52E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | 5:1 | MD-P2P | Insosafrole | 4676-39-5 | 5.49E+02 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | Piperonal | 120-57-0 | 6.52E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | 10:1 | MD-P2P | Insosafrole | 4676-39-5 | 6.52E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | Piperonal | 120-57-0 | 6.52E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | 5:1 | MD-P2P | Insosafrole | 4676-39-5 | 1.37E+03 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | Piperonal | 120-57-0 | 6.52E+01 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | MDMA | NA | 5.07E+00 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | MD-P2P | NA | 5.49E+02 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | Piperonal | 120-57-0 | 6.52E+03 | 83 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| | | Methamphetamine | 537-46-2 | 3.28E+05 | 0 | 4.79E-03 | 2.09E+02 | 2.09E+02 | | | |
| Unknown mixture | Methamphetamine | | | | | | | | | | | |
| Williams and Johnston [17] | Cotton balls were spiked with target odor and placed in a can. | Allyl sulfide | 592-88-1 | 6.01E+05 | > 80% | 6.01E+05 | 1.66E-06 | | | | 4.22E-08 |
| | | Cumene | 98-82-8 | 5.68E+05 | > 80% | 5.68E+05 | 2.40E-02 | 1.76E-06 | 4.17E+01 | 1.35E-06 | 4.22E-08 |
| | | dimethylthiazole | 541-58-2 | 7.39E+05 | > 80% | 7.39E+05 | 2.37E+07 | | | | |
| | | α-pinene | 80-56-8 | 4.99E+05 | > 80% | 6.92E-01 | 7.21E-05 | 2.00E-06 | 1.45E+00 | 1.39E-06 | |
| | | benzaldehyde | 100-52-7 | 7.80E+05 | > 80% | 7.80E+05 | 3.00E-03 | 2.60E+08 | 1.28E-06 | 3.33E+02 | 3.85E-09 |
Table 2 (continued)

| REF | Method | Mixture ratio | Compound  | CAS     | Conc. tested (ppm) | % of canines alerted | Canine ODT (ppm) | Human ODT (ppm) | ODTc:ODTh | Canine OAV of 1 ppm | Human OAV of 1 ppm | OAVc:OAVH |
|-----|--------|--------------|----------|---------|--------------------|---------------------|------------------|----------------|-----------|---------------------|------------------|-----------|
|     |        |              | Menthol  | 89-78-1 | 4.51E+05           | > 80%               | 4.51E+05         | 4.17E-02       | 1.08E+07  | 2.22E-06           | 2.40E+01         | 9.24E-08  |
|     |        |              | Cyclohexanone | 108-91-1 | 7.65E+05           | > 80%               | 7.65E+05         | 7.08E-01       | 1.08E+06  | 1.31E-06           | 1.41E+00         | 9.25E-07  |
|     |        |              | Eucalyptol | 470-82-6 | 4.74E+05           | > 80%               | 4.74E+05         | 1.62E-02       | 2.93E+07  | 2.11E-06           | 6.17E+01         | 3.42E-08  |
|     |        |              | Pentanethiol | 110-66-7 | 6.39E+05           | > 80%               | 6.39E+05         | 1.20E-04       | 5.31E+09  | 1.57E-06           | 8.32E+03         | 1.88E-10  |
|     |        |              | Toluene   | 108-88-3 | 7.48E+05           | > 80%               | 7.48E+05         | 1.55E+00       | 4.83E+05  | 1.34E-06           | 6.45E-01         | 2.07E-06  |

REF = reference; MD-P2P = 3,4-methylenedioxyphenyl-2-propanone; Mixture ratio = ratio of MD-P2P to Piperonal; ODT = odor detection threshold; OAV = odor activity value; ODTc = canine odor detection threshold; ODTh = human odor detection threshold; OAVc = odor activity value for canines; OAVH = odor activity value for humans. *Volume of can was not specified. In this table the can dimensions were assumed to be a cylinder of radius 5.08 cm, 4.62 cm height, displaced volume of cotton balls was not accounted for. All gas phase calculations assumed 1 atm at 25 °C.
Table 3
Summary of VOCs emitted from all illicit marijuana samples (sample code A and B in Section 1.5) and Sigma Pseudo™ Narcotic Scent Marijuana formulation (sample code C in Section 1.5) and sampled over 1 h at room temperature. Sigma Pseudo™ Narcotic Scent Marijuana formulation is indicated by underlined fonts.

| Compound                   | CAS    | RT (min) | Published descriptors | Published ODT (ppm) | Sample 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         | 2: 43 42       | 66          | 2.12E +06 | 2.49E +03 |
|                           |        |          |                       |                    | A 4         | 2: 43 42       | 65          | 3.37E +06 | 3.96E +03 |
|                           |        |          |                       |                    | A 7         | 2: 44 43       | 89          | 8.62E +03 | 1.01E +01 |
|                           |        |          |                       |                    | B 1         | 2: 44 43       | 66          | 3.75E +06 | 4.40E +03 |
|                           |        |          |                       |                    | B 4         | 2: 44 45 129 43| 66          | 1.86E +06 | 2.18E +03 |
|                           |        |          |                       |                    | C 1         | 2: 44 45 46   | 66          | 1.35E +06 | 1.59E +03 |
|                           |        |          |                       |                    | C 2         | 2: 43 43       | 85          | 2.14E +05 | 2.51E +02 |
|                           |        |          |                       |                    | C 3         | 4: 44 46 43 131| 67          | 1.36E +06 | 1.60E +03 |
| +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         | 13: 43 41 57 72 39 55 56 38| 84          | 2.02E +07 | 2.02E +06 |
|                           |        |          |                       |                    | A 2         | 11: 43 42 41 57 72 40 53 51 38| 85          | 1.47E +07 | 1.47E +06 |
|                           |        |          |                       |                    | A 3         | 5: 57 42 43 41 39| 67          | 2.03E +04 | 2.03E +03 |
|                           |        |          |                       |                    | A 4         | 10: 43 42 41 39 72 55 50 73| 84          | 7.18E +06 | 7.18E +05 |
|                           |        |          |                       |                    | A 5         | 4: 43 39 56 42| 88          | 4.16E +04 | 4.16E +03 |
|                           |        |          |                       |                    | A 6         | 10: 43 42 41 57 39 72 55 56| 85          | 2.94E +06 | 2.94E +05 |
|                           |        |          |                       |                    | A 7         | 71 58          | 73 37       | 2.20E +06 | 2.20E +05 |
|                           |        |          |                       |                    | B 1         | 14: 43 42 41 57 39 72 55 55 55| 85          | 7.00E +05 | 7.00E +04 |
|                           |        |          |                       |                    | B 2         | 71 50 70 53 38 37| 84          | 7.00E +05 | 7.00E +04 |
| +Acetaldehyde             | 75-07-0| 1.27     | Pungent, Ether        | Pungent, Ethereal, Aldehyde, Fruity| 1.50E-02| 1.86E-01      | 84          | 2.49E +04 | 2.49E +03 |
|                           |        |          |                       |                    | B 4         | 4: 43 42 41 39| 88          | 6.45E +04 | 6.45E +03 |
|                           |        |          |                       |                    | 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         | 7: 42 41 72 53 55 56 38| 84          | 6.11E +03 | 3.28E +04 |
|                           |        |          |                       |                    | B 3         | 4: 43 42 41 39| 96          | 2.85E +04 | 1.53E +05 |
|                           |        |          |                       |                    | B 4         | 4: 42 43 57 72| 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 | 1.98E +04 |
|                           |        |          |                       |                    | B 4         | 2: 101 103     | 81          | 1.72E +04 | 1.72E +03 |
| Compound                  | CAS     | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC | OAV |
|---------------------------|---------|----------|-----------------------|---------------------|-------------|--------|-------------|-----|-----|
| 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    |     |     |
|                           |         |          |                       |                     | A 5         | 1: 41    | 70  | 5.22E+04    |     |     |
|                           |         |          |                       |                     | A 6         | 3: 43 42 39 | 81  | 2.30E+04    |     |     |
| Ethylenimine              | 151-56-4| 1.30     |                       |                     | 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    |     |     |
| + Ethyl ether             | 60-29-7 | 1.31     | Ethereal              |                     | A 4         | 3: 39 53 51 | 85  | 3.34E+04    |     |     |
| Ketene                    | 463-51-4| 1.31     |                       |                     | A 7         | 1: 67     | 71  | 1.73E+04    |     |     |
|                           |         |          |                       |                     | B 1         | 3: 67 53 65 | 69  | 2.08E+04    |     |     |
|                           |         |          |                       |                     | B 3         | 1: 67      | 77  | 4.59E+03    |     |     |
| Isoprene                  | 78-79-5 | 1.33     |                       |                     | B 4         | 5: 67 41 53 66 | 95  | 7.61E+04    |     |     |
| (E)-1,3-Pentadiene        | 2004-70-8| 1.34    |                       |                     | C 2         | 3: 67 39 53 | 81  | 1.42E+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   |     |     |
|                           |         |          |                       |                     | 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         | 67  | 2.96E+04  1.35E+03   |     |     |
|                           |         |          |                       |                     | B 4         | 94         |     | 2.13E+04    |     |     |
| 4-methyldecane            | 2847-72-5| 1.39    |                       |                     | A 1         | 12: 43 42 71 41 57 39 70 55 56 | 66  | 2.55E+06  |     |     |
|                           |         |          |                       |                     | A 2         | 13: 43 71 42 41 57 39 56 86 | 66  | 2.66E+06  |     |     |
|                           |         |          |                       |                     | A 3         | 17: 43 42 41 70 86 56 50 40 57 | 65  | 4.43E+06  |     |     |
|                           |         |          |                       |                     | A 4         | 38 63 63 51 69 37 85 67 | 75  | 1.66E+04  |     |     |
|                           |         |          |                       |                     | A 5         | 66         |     | 1.35E+06    |     |     |
| Chemical Name                  | CAS Number | Characteristic | 10: | 9: | 8: | 7: | 6: | 5: | 4: | 3: | 2: | 1: |
|--------------------------------|------------|----------------|-----|----|----|----|----|----|----|----|----|----|
| 2-methylpentane               | 107-83-5   | 1.39           | 52  | 67 |    |    |    |    |    |    |    |    |
| 3,4,5-trimethyl-1-hexene      | 56728-10-0 | 1.39           | 56  | 40 | 12 | 72 | 70 | 86 | 56 | 40 | 65 | 50 |
| +γ-butyrolactone              | 96-48-0    | 1.40           | 39  | 55 | 41 | 86 | 53 | 69 | 38 | 52 | 67 |    |
| Acrylic acid                  | 79-10-7    | 1.40           | 2.95E-01 |    |    |    |    |    |    |    |    |    |
| 2,3,4-trimethylpentane        | 565-75-3   | 1.40           | 72  | 55 | 39 |    |    |    |    |    |    |    |
| 3-methylpentane               | 96-14-0    | 1.45           | 39  | 55 | 41 | 86 | 53 | 69 | 38 | 52 | 67 |    |
| 2-methylaziridine             | 75-55-8    | 1.45           | 39  | 55 | 41 | 86 | 53 | 69 | 38 | 52 | 67 |    |

S. Rice, J.A. Koziel / Data in Brief 5 (2015) 653–706
| Compound                  | CAS     | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models       | Net % match | PAC | OAV  |
|---------------------------|---------|----------|-----------------------|---------------------|-------------|--------------|-------------|-----|------|
| Isocyanatomethane         | 624-83-9| 1.46     | Flavornet [7]         |                     |             | B 4 2: 57 56 | 80          | 5.56E+04 |      |
|                           |         |          | TGSC [8]              |                     |             | A 3 2: 57 39 | 80          | 1.20E+04 |      |
|                           |         |          |                       |                     |             | A 4 2: 57 39 | 80          | 5.01E+04 |      |
|                           |         |          |                       |                     |             | A 6 2: 57 39 | 80          | 1.03E+05 |      |
|                           |         |          |                       |                     |             | A 7 2: 57 39 | 80          | 1.22E+05 |      |
| Cyanogen chloride         | 506-77-4| 1.47     | LRI and Odor [6]      |                     |             | B 1 2: 57 56 | 79          | 7.68E+03 |      |
| 1,2-dichloro-, (2)-ethene| 156-59-2| 1.47     | Devos et al. [5]      |                     |             | B 1 2: 57 56 | 79          | 7.77E+03 |      |
|                           |         |          |                       |                     |             | B 2 2: 56 57 | 79          | 1.20E+03 |      |
| +Furan                   | 110-00-9| 1.47     | Ethereal              |                     |             | B 1 2: 57 56 | 79          | 1.20E+03 |      |
| 1,1-dichloro ethene      | 75-35-4 | 1.47     |                       |                     |             | B 2 2: 56 57 | 79          | 1.20E+03 |      |
| +Dimethylsulfide         | 75-18-3 | 1.51     | Cabbage, Sulfur, Sulfur, Onion, Sweet corn, Vegetable, Cabbage, Tomato, Green, Radish | 2.24E-03 | A 2 3: 47 39 35 | 66          | 5.52E+04 | 2.47E+07 |      |
| Carbon disulfide         | 75-15-0 | 1.52     |                       |                     |             | A 4 4: 76 39 86 59 | 82          | 6.35E+04 | 6.65E+05 |      |
| +3-pentanone             | 96-22-0 | 1.53     | Ether                 |                     |             | A 4 2: 57 86 | 74          | 9.06E+04 | 2.86E+05 |      |
| +Butane                  | 106-97-8| 1.57     |                       |                     |             | A 6 2: 57 86 | 74          | 9.06E+04 | 2.86E+05 |      |
| Hordenine                | 539-15-1| 1.57     |                       |                     |             | A 3 5: 41 59 44 37 60 | 84          | 1.88E+06 | 9.21E+03 |      |
| +Propanal                | 123-38-6| 1.59     | Solvent, Earthy, Alcoholic, Wine, Whiskey, Cocoa, Nutty | 1.00E-02 | A 1 1: 58 | 66          | 3.41E+04 |      |      |
| Substance                                                                 | CAS Registry Number | Melting Point |
|--------------------------------------------------------------------------|---------------------|---------------|
| 1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide | 1447-71-8           | 1.61          |
| +Acetone                                                                 | 67-64-1             | 1.66          |
| +Acetic anhydride                                                        | 108-24-7            | 1.70          |
| Isobutyraldehyde                                                        | 78-84-2             | 1.76          |
| Compound                | CAS     | RT (min) | Published descriptors                  | Published ODT (ppm) | Sample code | Models          | Net % match | PAC  | OAV |
|-------------------------|---------|----------|---------------------------------------|---------------------|-------------|----------------|-------------|------|-----|
| +Methyl acetate         | 79-20-9 | 1.77     | Ethereal                              |                     |             |                |             |      |     |
| Cyclohexene             | 110-83-8| 2.02     |                                       |                     |             |                |             |      |     |
| Methacrolein            | 78-85-3 | 2.14     | Wild hyacinth foliage                 |                     |             |                |             |      |     |
| +Butyraldehyde          | 123-72-8| 2.16     | Pungent, Cocoa, Musty, Green, Malty, Bread|                     |             |                |             |      |     |
| +2-butenal              | 4170-30-3| 2.31     | Flower                                |                     |             |                |             |      |     |
| methylhydrazine         | 60-34-4 | 2.32     |                                       |                     |             |                |             |      |     |
| Diazomethane            | 334-88-3| 2.33     |                                       |                     |             |                |             |      |     |
| +Isopropyl alcohol      | 67-63-0 | 2.33     | Alcohol, Musty, Woody                |                     |             |                |             |      |     |
| +Formic acid            | 64-18-6 | 2.33     | Acetic                                |                     |             |                |             |      |     |
| Nitrogen dioxide        | 10102-44-0 | 2.34     |                                       |                     |             |                |             |      |     |
| +Ethanol                | 64-17-5 | 2.34     | Sweet, Alcoholic                      |                     |             |                |             |      |     |
| Compound                  | CAS Number | pKa | Sensory Descriptions                                              | pH | µM | 2.92E-04 | 9.77E-04 | 1.56E-04 | 4.68E-01 | 3.39E-00 | 7.77E-00 | 1.87E+00 |
|---------------------------|------------|-----|-----------------------------------------------------------------|----|----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Methylene chloride        | 75-09-2    | 2.42|                                                                 |    |    | 2.82E+01 | 2.91E+01 | 3.01E+01 | 3.43E+01 | 3.78E+01 | 4.68E+01 | 5.86E+03 |
| Amitrole                  | 61-82-5    | 2.44|                                                                 |    |    | 8.85E+04 | 7.19E+04 | 2.92E+04 | 1.30E+07 | 1.04E+04 | 1.92E+03 | 1.96E+04 |
| Allyl alcohol             | 107-18-6   | 2.75| Pungent, Mustard                                                 |    |    | 2.69E-01 | 7.77E+01 | 1.94E+04 | 7.19E+04 | 1.04E+04 | 1.92E+03 | 1.96E+04 |
| + Methylbutanal           | 590-86-3   | 2.75| Malt, Ethereal, Aldehydic, Chocolate, Peach, Fatty              |    |    | 1.00E+00 | 2.24E-03 | 1.76E+05 | 6.23E+03 | 1.06E+04 | 5.92E+02 | 5.74E+03 |
| Allyl alcohol             | 107-18-6   | 2.75|                                                                 |    |    | 2.69E-01 | 1.08E+05 | 2.92E+04 | 1.30E+07 | 1.04E+04 | 1.92E+03 | 1.96E+04 |
| Acetonitrile              | 75-05-8    | 3.28|                                                                 |    |    | 9.77E-01 | 1.20E+05 | 1.20E+05 | 9.42E+02 | 1.20E+03 | 9.42E+02 | 9.42E+02 |
| Chloroform                | 67-66-3    | 3.78|                                                                 |    |    | 1.18E+05 | 1.20E+03 | 1.20E+03 | 9.42E+02 | 1.20E+03 | 9.42E+02 | 9.42E+02 |
| Propyl formate            | 110-74-7   | 3.91| Sweet, Ethereal, Green, Rum, Fruity, Berry                    |    |    | 3.39E+00 | 1.56E+05 | 4.59E+04 | 4.59E+04 | 4.59E+04 | 4.59E+04 | 4.59E+04 |
| Hydrazine                 | 302-01-2   | 3.92|                                                                 |    |    | 3.00E+00 | 2.35E+03 | 7.85E+02 | 7.85E+02 | 7.85E+02 | 7.85E+02 | 7.85E+02 |
| 3-pentanol                | 584-02-1   | 3.92| Fruit, Herbal                                                   |    |    | 4.68E-01 | 1.56E+05 | 4.59E+04 | 4.59E+04 | 4.59E+04 | 4.59E+04 | 4.59E+04 |
| + 1,1-dimethyl-hydrazine  | 57-14-7    | 3.92|                                                                 |    |    | 7.77E+00 | 1.87E+05 | 1.87E+05 | 1.87E+05 | 1.87E+05 | 1.87E+05 | 1.87E+05 |
| Compound                        | CAS       | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models        | Net % match | PAC   | OAV   |
|--------------------------------|-----------|----------|-----------------------|---------------------|-------------|---------------|-------------|-------|-------|
| Ethylenediamine                | 107-15-3  | 3.92     |                       |                     | B 4         | 9: 59 42 60 41 39 58 40 36 80 6.00E+05 | 7.94E+04 | 8.76E+04 |       |
|                                |           |          |                       |                     | A 1         | 79            |             |       |       |
|                                |           |          |                       |                     | A 2         | 75            |             |       |       |
|                                |           |          |                       |                     | A 3         | 71            | 2.81E+04   |       |       |
|                                |           |          |                       |                     | A 7         | 75            | 1.41E+05   |       |       |
|                                |           |          |                       |                     | B 1         | 75            | 1.01E+05   |       |       |
|                                |           |          |                       |                     | B 3         | 71            | 4.76E+05   |       |       |
|                                |           |          |                       |                     | B 4         | 79            | 5.13E+05   |       |       |
| tert-butanol                   | 75-65-0   | 3.93     | Camphor               |                     | A 2         | 70            | 1.53E+04   |       |       |
|                                |           |          |                       |                     | B 3         | 77            | 7.79E+05   |       |       |
|                                |           |          |                       |                     | B 4         | 74            | 2.14E+06   |       |       |
| Methyl formate                 | 107-31-3  | 3.93     | Fruity, Plum          | 9.33E+01            | A 1         | 1: 33         | 5.81E+03   | 6.22E+01 |       |
|                                |           |          |                       |                     | A 4         | 72            | 3.42E+03   | 3.67E+01 |       |
|                                |           |          |                       |                     | B 4         | 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 |       |
|                                |           |          |                       |                     | B 4         | 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         | 67            | 1.57E+04   |       |       |
| + Phenylethyl alcohol          | 60-12-8   | 5.06     | Floral                | 1.70E-02            | A 2         | 74            | 9.14E+04   | 5.38E+06 |       |
| + Toluene                      | 108-88-3  | 5.07     | Honey, Spice, Rose, Lilac | 1.55E+00            | A 1         | 81            | 1.39E+04   | 8.98E+03 |       |
|                                |           |          |                       |                     | A 2         | 96            | 9.14E+04   | 5.90E+04 |       |
| + Pentanal                     | 110-62-3  | 5.97     | Almond, Malt, Pungent, Grass, Tallow, Fat | 6.03E-03            | A 3         | 79            | 5.82E+04   | 3.76E+04 |       |
| + Hexanal                      | 66-25-1   | 5.99     | Green                 | 4.00E-03            | A 6         | 70            | 3.47E+04   | 5.76E+06 |       |
|                                |           |          |                       |                     | A 7         | 85            | 4.12E+04   | 2.98E+06 |       |
| Glutaraldehyde                 | 111-30-8  | 6.02     |                       |                     | B 3         | 73            | 2.30E+04   | 1.66E+06 |       |
|                                |           |          |                       |                     | B 1         | 69            | 1.15E+05   |       |       |
|                                |           |          |                       |                     | B 2         | 70            | 5.45E+05   |       |       |
| + 1-butanol                    | 71-36-3   | 6.09     | Medicine, Fruit       | 4.90E-01            | A 3         | 79            | 1.25E+05   | 2.54E+05 |       |
|                                |           |          |                       |                     | A 4         | 77            | 1.82E+04   | 3.72E+04 |       |
|                                |           |          |                       |                     | A 6         | 79            | 3.76E+04   | 7.67E+04 |       |
|                                |           |          |                       |                     | A 7         | 83            | 3.18E+04   | 6.48E+04 |       |
| Compound                     | CAS Number | Odor          | S. Rice, J.A. Koziel / Data in Brief 5 (2015) 653–766 |
|----------------------------|------------|---------------|-----------------------------------------------------|
| Butyl formate               | 592-84-7   | Fruity        |                                                     |
| + Isobutanol                | 78-83-1    | Wine, Solvent |                                                     |
| Propanoic acid, anhydride   | 123-62-6   | Bitter        |                                                     |
| 4-methyl-3-penten-2-one     | 141-79-7   | Sweet, Chemical | Pungent, Earthy, Vegetable, Acrylic | 5.62E-02 |
| 2,2’-Bioxirane              | 1464-53-5  | 6.66          |                                                     |
| α-angelica lactone          | 591-12-8   | 6.66          |                                                     |
| α-isoamyl alcohol           | 123-51-3   | 7.52          | Whiskey, Malt, Burnt Fusel oil, Alcoholic, Whiskey, Fruity, Banana | 4.47E-02 |
| Amyl alcohol                | 71-41-0    | 7.52          | Balsamic Fusel, Oil, Sweet, Balsam | 4.68E-01 |
| 2-isopropenyl-3-methylpyrazine | 145984-65-2 | 7.67        | Terpenic, Mint, Spice | Terpenic |
| α-phenlandrene              | 99-83-2    | 7.89          |                                                     |
| Compound | CAS       | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models   | Net % match | PAC  | OAV  |
|----------|-----------|----------|-----------------------|---------------------|-------------|----------|-------------|------|------|
|          |           |          | Flavornet [7] | TGSC [8] | LRI and Odor [6] | Devos et al. [5] |            |      |      |
| α-pinene | 80-56-8   | 7.90     | Pine, Herbal, Turpentine | 6.92E-01 | C 1 | 90 | 8.81E+04 | 3.75E+04 |
|          |           |          |                       |                     | C 2 | 86 | 8.42E+04 | 8.80E+06 |
|          |           |          |                       |                     | C 3 | 89 | 8.41E+04 | 3.08E+05 |
|          |           |          |                       |                     | A 1 | 93 | 1.05E+06 | 1.52E+06 |
|          |           |          |                       |                     | A 2 | 97 | 6.09E+06 | 8.80E+06 |
|          |           |          |                       |                     | A 3 | 92 | 2.14E+05 | 3.08E+05 |
|          |           |          |                       |                     | A 5 | 93 | 3.65E+05 | 5.28E+05 |
|          |           |          |                       |                     | A 6 | 93 | 1.61E+05 | 2.33E+05 |
|          |           |          |                       |                     | A 7 | 97 | 4.88E+05 | 7.05E+05 |
|          |           |          |                       |                     | B 1 | 98 | 1.79E+06 | 2.58E+06 |
|          |           |          |                       |                     | B 2 | 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 | 70 | 8.42E+04 | 1.22E+05 |
| Betahistine | 5638-76-6 | 7.90     |                       |                     | A 1 | 65 | 2.02E+07 | 1.04E+04 |
|          |           |          |                       |                     | A 2 | 69 | 4.37E+04 | 1.04E+04 |
|          |           |          |                       |                     | A 3 | 67 | 1.03E+04 | 1.04E+04 |
|          |           |          |                       |                     | A 4 | 70 | 5.56E+05 | 5.42E+04 |
|          |           |          |                       |                     | C 1 | 73 | 4.42E+05 | 5.42E+04 |
|          |           |          |                       |                     | C 2 | 68 | 5.61E+05 | 5.42E+04 |
|          |           |          |                       |                     | C 3 | 67 | 1.29E+06 | 5.42E+04 |
|          |           |          |                       |                     | B 1 | 67 | 1.29E+06 | 5.42E+04 |
|          |           |          |                       |                     | B 2 | 69 | 5.94E+03 | 5.42E+04 |
| Conessine | 546-06-5  | 8.31     |                       |                     | B 3 | 69 | 5.94E+03 | 2.02E+07 |
| 2-formyl pyrrole | 1003-29-8 | 9.09     | Musty, Beefy, Coffee |                     | B 4 | 74 | 5.31E+04 | 2.02E+07 |
| 1,4-dimethoxybenzene | 150-78-7 | 9.19     | Sweet, Green, New mown hay, Fennel |                     | B 5 | 74 | 5.31E+04 | 2.02E+07 |
| + α-ionol | 25312-34-9 | 9.20     | Ionone, Tropical, Sweet, Floral, Violet, Woody |                     | B 6 | 73 | 2.42E+04 | 2.42E+04 |
| Menthy acetate | 16409-45-3 | 9.20     | Tea cooling, Minty, Fruity, Berry | 6.17E+00 | C 1 | 74 | 1.46E+05 | 2.37E+04 |
|          |           |          |                       |                     | C 2 | 79 | 5.85E+04 | 8.49E+04 |
| Compound                  | CAS  | MP  | Odor Notes                                | Pubchem Properties |
|---------------------------|------|-----|-------------------------------------------|--------------------|
| 4-methyl guaiacol         | 93-51-6 | 9.20 | Spicy                                     |                    |
| 2-acetyl-6-methyl pyrazine| 22047-26-3 | 9.26 | Roasted coffee, Cocoa, Popcorn            |                    |
| Tricyclene                | 508-32-7 | 9.30 |                                          |                    |
| 2-indanone                | 615-13-4 | 9.47 |                                          |                    |
| + Styrene                 | 100-42-5 | 9.48 | Balsamic, Gasoline                        | 1.45E-01           |
| β-pinene                  | 18172-67-3 | 9.90 | Pine, Resin, Terpenic, Turpentine         |                    |
| DL-menthol                | 89-78-1 | 10.34| Peppermint, Cool, Woody                  | 4.17E-02           |
| +(-)-menthol              | 1490-04-6 | 10.34| Minty                                     | 4.17E-02           |
| +o-dimethyl hydroquinone  | 91-16-7 | 10.34| Vanilla                                   |                    |
| Compound                     | CAS          | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC | OAV |
|------------------------------|--------------|----------|-----------------------|--------------------|-------------|--------|-------------|-----|-----|
| (+)-carvomenthene            | 1195-31-9    | 10.34    |                       |                    |             |        |             |     |     |
| Menthol                      | 15356-70-4   | 10.36    |                       | 4.17E-02           |             |        |             |     |     |
| 2,4,6-trimethylphenol        | 527-60-6     | 10.48    | Phenolic              |                    |             |        |             |     |     |
| +α-terpinene                 | 99-86-5      | 10.50    | Lemon Woody           |                    |             |        |             |     |     |
| (±)-4-Carene                 | 29050-33-7   | 10.50    |                       | 4.00E+00           |             |        |             |     |     |
| Furfurylmethylamphetamine   | 13445-60-8   | 10.50    |                       |                    |             |        |             |     |     |
| +Phenylacetic acid           | 103-82-2     | 10.53    | Honey, Flower         |                    |             |        |             |     |     |

9: 95 94 138 96 123 67 53 81
79

C 1 85 1.01E+05
C 2 85 8.21E+04
C 3 86 1.90E+05
C 4 66 8.02E+04 1.92E+06

Flavornet [7]
TGSC [8]
LRI and Odor [6]
Devos et al. [5]
| Chemical Name                  | CAS Number | Mass  | Subcategory           | pK<sub>α</sub> | A  | 87  | 5.03E+04 | 1.15E+06 | 1.33E+05 |
|-------------------------------|------------|-------|-----------------------|---------------|----|-----|----------|----------|----------|
| 1-hexanol                     | 111-27-3   | 10.73 | Resin, Flower, Breen  | 4.37E-02      | A  | 6   | 87       | 5.03E+04 | 1.15E+06 |
| Diacetone alcohol             | 123-42-2   | 10.78 |                       | 8.91E-01      | A  | 7   | 77       | 5.51E+04 | 6.18E+04 |
| (1R)-(−)-trans-isolimonene    | 5113-87-1  | 10.85 |                       |               | B  | 3   | 87       | 2.54E+05 | 2.85E+05 |
| 2,2,5-trimethylhexane + Limonene | 3522-94-9 | 10.88 | Lemon, Orange Citrus  | 1.00E-02      | A  | 4   | 80       | 1.28E+05 | 7.64E+07 |
| + Camphene                    | 79-92-5    | 10.93 | Camphor Woody         |               | A  | 6   | 87       | 2.06E+05 | 4.71E+05 |
| + Limonene                    | 138-86-3   | 10.89 |                       | 4.37E-01      | A  | 1   | 95       | 3.33E+07 | 7.64E+07 |
| + Limonene                    | 138-86-3   | 10.89 |                       | 4.37E-01      | A  | 2   | 95       | 2.21E+07 | 5.05E+07 |
| + Limonene                    | 138-86-3   | 10.89 |                       | 4.37E-01      | A  | 3   | 95       | 1.97E+06 | 4.51E+06 |
| + Limonene                    | 138-86-3   | 10.89 |                       | 4.37E-01      | A  | 4   | 95       | 4.35E+05 | 9.97E+05 |
| + Camphene                    | 79-92-5    | 10.93 |                       |               | A  | 5   | 95       | 4.38E+05 | 7.26E+05 |
| + Camphene                    | 79-92-5    | 10.93 |                       |               | A  | 6   | 87       | 1.62E+05 | 3.71E+05 |
| + Camphene                    | 79-92-5    | 10.93 |                       |               | A  | 7   | 87       | 3.86E+04 | 8.84E+04 |

S. Rice, J.A. Koziel / Data in Brief 5 (2015) 653–706
| Compound                      | CAS     | RT (min) | Published descriptors          | Published ODT (ppm) | Sample code | Models | Net % match | PAC | OAV |
|-------------------------------|---------|----------|--------------------------------|---------------------|-------------|--------|-------------|-----|------|
| +p-cymene                     | 99-87-6 | 11.36    | Solvent, Gasoline, Citrus      |                     |             |        |             |     |      |
| Eucalyptol                    | 470-82-6| 10.97    | Mint, Sweet Eucalyptus, Herbal, Camphor | 1.62E-02           |             |        |             |     |      |
| N-Benzyl-2-phenethylamine     | 3647-71-0| 11.32    |                                 |                     |             |        |             |     |      |
| Phenyl propane                | 103-65-1| 11.32    |                                 |                     |             |        |             |     |      |
| 3-ethyl-o-xylene              | 933-98-2| 11.35    |                                 |                     |             |        |             |     |      |
| m-cymene                      | 535-77-3| 11.36    |                                 |                     |             |        |             |     |      |

Table 3 (continued)
1,2,3,4-tetramethylbenzene 488-23-3 11.36 Gasoline, Sweet 2.63E-02

1-ethyl-2,4-dimethylbenzene 874-41-9 11.36

1-phenyl-1-decanone 6048-82-4 11.40

N,N-dimethylbenzenamine 121-69-7 11.40

Isodurene 527-53-7 11.40

1-(3-methylphenyl)-ethanone 585-74-0 11.41

Dihydromethylcyclopentapyrazine 23747-48-0 11.41 Roast, Nut Earthy, Baked potato, Peanut, Roasted

1-ethyl-3,5-dimethylbenzene 934-74-7 11.46
| Compound                    | CAS       | RT (min) | Published descriptors | Published ODT (ppm) | Models          | Sample code | Net % match | PAC     | OAV     |
|-----------------------------|-----------|----------|-----------------------|---------------------|-----------------|-------------|-------------|---------|---------|
| +Methylisohexenyl ketone    | 110-93-0  | 11.51    | Pepper, Mushroom,     |                     |                 |             |             |         |         |
|                             |           |          | Citrus                |                     |                 |             |             |         |         |
| 4-ethyl-1,2-dimethylbenzene | 934-80-5  | 11.57    | Citrus                |                     |                 |             |             |         |         |
| +5-3-carene                 | 13466-78-9| 11.57    | Lemon, Resin          |                     |                 |             |             |         |         |
| Sabinene                    | 3387-41-5 | 11.59    | Pepper, Turpentine,   |                     |                 |             |             |         |         |
|                             |           |          | Wood                  |                     |                 |             |             |         |         |
| Name                                      | CAS No. | Boiling Point (°C) | Comments                      | Remarks                      |
|-------------------------------------------|---------|--------------------|-------------------------------|------------------------------|
| γ-terpinene                               | 99-85-4 | 11.79              | Gasoline, Terpenic Turpentine |                             |
| +Terpinolene                              | 586-62-9| 11.83              | Pine, Plastic Herbal          | 2.00E-01                     |
| Ethyl benzene                             | 100-41-4| 11.84              |                               | 2.88E+00                     |
| Acetic acid                               | 64-19-7 | 12.23              | Sour Acidic                   | 1.45E-01                     |
| N-methyl-N-nitroso urea                   | 684-93-5| 12.26              |                               | 8.16E+01                     |
| (z)-rose oxide                            | 16409-43-1| 12.28             | Green, Red rose, Spic, Fresh geranium |                   |
| Phenetole                                 | 103-73-1| 12.52              |                               | 1.18E+05                     |
| 2-hydroxyacetophenone                     | 118-93-4| 12.53              | Phenolic                      |                             |
| 1-methyl-2-propyl benzene                 | 1074-17-5| 12.63             |                               |                             |
| 2-phenyl propionaldehyde                  | 93-53-8 | 12.63              | Fresh, Sharp, Green, Hya- cinth, Leaf, Lilac |                   |
Table 3 (continued)

| Compound                      | CAS      | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC | OAV |
|-------------------------------|----------|----------|-----------------------|---------------------|-------------|--------|-------------|-----|-----|
| +o-xylene                    | 95-47-6  | 13.07    | Geranium              | 8.51E-01            | A 2         | 5: 77 134 106 119 52 | 73  | 9.60E+04 | 1.13E+05 |
| +p-xylene                    | 106-42-3 | 13.08    | Geranium              | 4.90E-01            | A 2         | 81     | 4.01E+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 | 1.31E+06 |
|                              |          |          |                       |                     | C 1         | 19: 81 41 53 55 79 39 82 91 80 | 98  | 1.36E+06 | 1.46E+07 |
|                              |          |          |                       |                     |             | 137 67 70 42 105 123 85 38 |     |       |
|                              |          |          |                       |                     |             | 153 77 |     |       |
|                              |          |          |                       |                     |             | 13: 153 152 80 55 77 78 91 42 | 99  | 1.43E+06 | 1.51E+07 |
|                              |          |          |                       |                     |             | 71 66 52 40 123 |       |       |
|                              |          |          |                       |                     |             | 20: 81 69 152 67 80 41 66 68 | 98  | 1.50E+06 | 1.67E+06 |
|                              |          |          |                       |                     |             | 82 39 109 72 91 52 55 137 97 |     |       |
| Linalool oxide               | 5989-33-3| 13.67    | Flower, Wood          | 1.91E+05            | A 5         | 11: 207 266 83 70 79 55 112 | 65  | 8.06E+04 | 9.99E+04 |
|                              |          |          | Earthy, Floral, Sweet, Woody |       |             | 67 85 53 97 | 83  | 3.23E+05 |       |
|                              |          |          |                       |                     | A 6         | 19: 93 55 111 70 92 71 94 43 | 80  | 3.07E+05 |       |
|                              |          |          |                       |                     | A 7         | 67 81 83 68 91 69 84 74 57 |     |       |
|                              |          |          |                       |                     |             | 137 82 |     |       |
|                              |          |          |                       |                     |             | 137 82 |     |       |
|                              |          |          |                       |                     |             | 119 77 120 82 135 51 39 |     |       |
| 1,3-diethylbenzene           | 141-93-5 | 13.81    |                       | 8.43E+04            | A 2         | 14: 105 93 94 137 81 53 65 | 68  | 3.07E+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 | 3.18E+06 |
|                              |          |          |                       |                     | 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                 | 8.43E+04            | A 6         | 4: 70 55 39 82 | 67  | 1.34E+04 |       |
| Tranylcypromine              | 155-09-9 | 13.91    |                       | 1.31E+06            | A 2         | 7: 132 117 102 118 91 115 99 | 69  | 1.31E+06 |       |
| +Propanoic acid              | 79-09-4  | 13.91    | Pungent, Rancid, Soy  | 3.55E-02            | A 6         | 3: 73 74 60 | 65  | 1.76E+05 | 4.97E+06 |
| 5-methylindane               | 874-35-1 | 13.91    |                       | 2.94E+05            | A 1         | 5: 132 116 39 131 57 | 88  | 2.94E+05 |       |
|                              |          |          |                       |                     | A 2         | 5: 132 116 39 131 57 | 88  | 2.94E+05 |       |
|                              |          |          |                       |                     | B 1         | 5: 91 132 115 116 64 | 78  | 4.44E+04 |       |
| 2-ethenyl-1,3-dimethylbenzene| 2039-90-9| 13.91    |                       | 1.31E+06            | 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 |       |
| Compound                        | CAS     | Boiling Point | Properties                       | Sensory Profile                      |
|--------------------------------|---------|---------------|----------------------------------|--------------------------------------|
| Propylene glycol               | 57-55-6 | 13.98         |                                 |                                      |
| Indane                         | 496-11-7| 13.98         |                                 |                                      |
| 2-chloroacetophenone           | 532-27-4| 14.09         | Apple blossom                    |                                      |
| + Benzaldehyde                 | 100-52-7| 14.09         | Almond, Fruity, Burnt sugar      |                                      |
| + Ethyl lactate                | 97-64-3 | 14.10         | Fruit, Sharp, Tart, Fruity, Buttery, Butterscotch |                                      |
| Isobutyrophenone               | 611-70-1| 14.10         | Green                            |                                      |
| Dimethyl octanol               | 106-21-8| 14.11         | Waxy, Soapy, Aldehydic, Leathery, Musty, Citrus, Green |                                      |
| 1-Dodecanol                    | 112-53-8| 14.11         | Fat, Wax, Earthy, Soapy, Waxy, Fatty, Honey, Coconut |                                      |
| + 1-Decanol                    | 112-30-1| 14.11         | Fat, Fatty, Waxy, Floral, Orange, Sweet, Clean, Watery |                                      |
| 1-Nonanol                       | 143-08-8| 14.12         | Fat, Green, Fresh, Clean, Fatty, Floral, Rose, Orange, Dusty, Wet, Oily |                                      |
| + Undecane                     | 1120-21-4| 14.13        | Alkane                           |                                      |
| + Nonane                       | 111-84-2| 14.13        | Alkane, Gasoline                 |                                      |
| + Dodecane                     | 112-40-3| 14.13        | Alkane                           |                                      |
| + Tridecane                    | 629-50-5| 14.14        | Alkane                           |                                      |
| 2,2-dimethylbutane             | 75-83-2 | 14.15        |                                 |                                      |
Table 3 (continued)

| Compound                        | CAS      | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models       | Net % match | PAC  | OAV  |
|---------------------------------|----------|----------|-----------------------|---------------------|-------------|--------------|-------------|------|------|
| 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 | 81  | 1.39E+06 |
|                                 |          |          |                       |                     |             | 80 41 106 107 39 43 94 120  | 115 52 135 67 54 |
| 3-(1-methylethyl)-phenol methylcarbamate | 64-00-6  | 14.20    |                       |                     | A 1         | 8: 121 105 136 106 91 77 79 | 76  | 7.43E+05 |
|                                 |          |          |                       |                     | A 2         | 13: 105 121 51 79 136 77 78 | 74  | 7.94E+05 |
|                                 |          |          |                       |                     | A 4         | 53 103 106 39 120 43       |     |       |
|                                 |          |          |                       |                     | A 7         | 13: 121 78 136 68 103 117 80 | 66  | 3.18E+05 |
|                                 |          |          |                       |                     |             | 52 51 77 106 107 81       |     |       |
| Acetone cyanohydrin             | 75-86-5  | 14.27    |                       |                     | B 1         | 3: 136 91 107           | 74  | 4.44E+04 |
|                                 |          |          |                       |                     | 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         | 9: 120 55 115 93 135 52 108 | 85  | 5.16E+05 |
|                                 |          |          |                       |                     | A 2         | 103 133                |     |       |
| o-cymene                        | 527-84-4 | 14.47    |                       |                     | A 2         | 18: 91 52 119 106 134 93 55 | 88  | 4.83E+05 |
|                                 |          |          |                       |                     |             | 105 92 115 103 117 79 65 120 | 63 133 116 |
| 1,2-diethylbenzene              | 135-01-3 | 14.47    |                       |                     | A 1         | 18: 91 52 119 106 134 93 55 | 88  | 4.95E+04 |
|                                 |          |          |                       |                     | A 2         | 105 92 115 103 117 79 65 120 | 84  | 8.70E+05 |
| p-tert-butylphenol              | 98-54-4  | 14.48    | Leathery              |                     | A 7         | 1: 121 77 55 136 67 120 79 | 68  | 1.54E+04 |
| tert-butyl-benzene              | 98-06-6  | 14.48    | Leathery              |                     | A 1         | 7: 122 105 103 93 121 51 57 | 89  | 6.59E+04 |
|                                 |          |          |                       |                     | A 2         | 86                    |     | 3.38E+05 |
| o-methylacetophenone            | 577-16-2 | 14.48    | Floral                | 6.61E-03            | A 1         | 3: 91 120 134           | 76  | 6.51E+04 |
| 2-methoxethanol                 | 109-86-4 | 14.62    |                       |                     | A 6         | 2: 43 55               | 65  | 1.39E+05 |
| +2-Butanol                      | 78-92-2  | 14.66    | Wine                  | 1.70E+00            | C 2         | 13: 45 43 47 44 55 46 42 54 | 69  | 2.96E+07 |
|                                 |          |          | Sweet, Apricot        |                     |             | 60 58 76 38 86          |     | 1.74E+07 |
| Maltol                          | 118-71-8 | 14.67    | Caramel               | 6.61E-03            | A 4         | 3: 98 126 71            | 66  | 5.65E+03 |
|                                 |          |          | Sweet, Caramel, Cotton candy, Jam, Fruity, Baked | | | | | | |
| Linalyl acetate                 | 115-95-7 | 15.09    | Sweet, Fruit          | 8.91E-03            | A 4         | 1: 121 77 55 136 67 120 79 | 77  | 2.39E+04 |
|                                 |          |          | Herbal                |                     | A 6         | 1: 83                   | 74  | 4.56E+04 |
| Geranyl butyrate                | 106-29-6 | 15.09    | Fruit, Rose, Waxy Apple |                | A 4         | 1: 83                   | 68  | 1.45E+04 |
| Substance                        | CAS Number | Aromatic Description       | Aromatic Value | Flavor Description                  |
|--------------------------------|------------|----------------------------|----------------|-------------------------------------|
| Isobornyl thiocyanate          | 115-31-1   | 15.11                      | A 1            | 20: 92 105 80 51 117 66 137 66 3.33E+07 |
|                                |            |                            | A 2            | 20: 68 93 67 94 136 59 107 91 2.21E+07 |
|                                |            |                            | A 3            | 9: 81 137 95 106 122 43 42 67 9.69E+05 |
|                                |            |                            | A 6            | 20: 55 65 77 93 39 41 136 80 7.74E+05 |
|                                |            |                            | A 7            | 20: 93 69 80 71 72 122 41 92 3.68E+05 |
|                                |            |                            | B 3            | 10: 72 139 94 65 70 57 67 92 1.18E+06 |
|                                |            |                            | B 3            | 10: 56 84 51 56 53 72 137 126 6.45E+05 |
| Linalyl propionate             | 144-39-8   | 15.11                      | A 1            | 3: 69 71 43 85 9.62E+04 1.79E+06 |
|                                |            | Fresh, Bergamot, Lily,     | A 2            | 89 1.00E+05 1.87E+06 |
|                                |            | Woody, Rose, Rum           | A 5            | 91 3.31E+05 6.16E+06 |
|                                |            |                            | A 6            | 96 8.95E+05 1.67E+06 |
|                                |            |                            | A 7            | 20: 93 69 80 71 72 122 41 92 3.68E+05 6.85E+06 |
|                                |            |                            | B 3            | 10: 56 84 51 56 53 72 137 126 6.45E+05 |
| Linalool                       | 78-70-6    | 15.12                      | A 1            | 3: 69 71 43 85 9.62E+04 1.79E+06 |
|                                |            | Flower, Lavender           | A 2            | 89 1.00E+05 1.87E+06 |
| 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 2            | 8: 21 168 67 1.48E+05 |
| cis-2-pinanol                  | 4948-29-2  | 15.41                      | C 3            | 3: 82 69 168 1.48E+05 |
|                                |            | Herbal                     | A 5            | 96 1.30E+04 |
|                                |            |                            | A 6            | 20: 81 99 79 97 121 67 77 43 95 8.31E+05 |
|                                |            |                            | B 3            | 10: 72 139 94 65 70 57 67 92 1.18E+06 2.19E+07 |
| trans-carveol                  | 1197-07-5  | 15.51                      | C 1            | 4: 94 93 58 72 79 1.66E+04 |
|                                |            | Caraway, Solvent,         | C 2            | 19: 109 106 43 137 67 119 69 94 1.36E+06 |
| β-cyclocitral                  | 432-25-7   | 15.52                      | C 1            | 20: 95 134 119 138 77 106 121 87 115 115 121 1.15E+06 |
|                                |            | Mint                      | C 2            | 20: 95 134 119 138 77 106 121 87 9.49E+05 |
|                                |            | Tropical, Saffron, Herbal, | C 3            | 152 137 67 107 41 79 65 91 78 8.54E+05 |
|                                |            | clean, Rose, Sweet, Tobacco, | C 4            | 152 137 67 107 41 79 65 91 78 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                      | A 1            | 76 4.88E+04 |
|                                |            | Camphor, Borneol, Pine,    | A 2            | 76 4.88E+04 |
|                                |            | Woody, Dry, Sweet, Lemon   | A 4            | 72 121 53 96 67 2.37E+05 |
| Compound | CAS      | RT (min) | Published descriptors                  | Published ODT (ppm) | Sample code | Models | Net % match | PAC OAV |
|----------|----------|----------|----------------------------------------|---------------------|-------------|--------|-------------|---------|
|          |          |          |                                       |                     |             | A 5    | 72          | 5.65E+04 |
|          |          |          |                                       |                     |             | 6      | 98          | 1.84E+06 |
| +1-methyl-1H-pyrrole | 96-54-8  | 15.72    | Smoky, Woody, Herbal                  | 1.29E-01            | 8           | 5      | 98          | 5.65E+04 |
| (-)-terpinen-4-ol | 20126-76-5 | 16.20    | Turpentine, Nutmeg, Menthol, Citrus, Terpiny, Spicy | 6.43E-04            | 3           | 95     | 77          | 6.59E+04 |
| 1-terpinen-4-ol   | 562-74-3  | 16.20    | Woody, Ceding, mentholic, Citrus, Terpiny, Spicy | 3.90E-04            | 8           | 77     | 109         | 6.59E+04 |
| Thujone           | 546-80-5  | 16.22    | Cedar leaf                             | 1.29E-01            | 2           | 77     | 8.49E+03    | 6.59E+04 |
| 2-Methyl-4-(1-methylethyl)-2-cyclohexenone | 41469-46-9 | 16.33    |                                       |                     |             | 6      | 98          | 1.94E+04 |
| Camphor           | 76-22-2   | 16.33    | Camphor                                | 5.13E-02            | 4           | 109    | 95          | 2.28E+06 |
| Pulegone          | 89-82-7   | 16.34    | Peppermint, Camphor, Fresh, Herbal, Buchu | 3.39E-03            | 3           | 109    | 95          | 2.67E+04 |
| 2,4,4-trimethylpentane | 540-84-1  | 16.57    |                                       |                     |             | 6      | 77          | 1.45E+04 |
| γ-hexalactone     | 695-06-7  | 17.20    | Coumarin, Sweet                        | 1.20E+06            | 6           | 81     | 8.39E+04    | 1.45E+04 |
| Borneol           | 507-70-0  | 17.60    | Camphor                                | 2.09E-03            | 6           | 139    | 96          | 1.45E+04 |
| Isobornyl acetate | 125-12-2  | 17.60    | Balsamic                               |                     |             | 6      | 3.89E+04    | 1.85E+07 |
| +Laevororne       | 464-45-9  | 17.60    | Pine, Woody, Camphor                  |                     |             | 6      | 7.58E+05    | 1.85E+07 |
| +α-terpineol      | 98-55-5   | 17.73    | Oil, Anise, Mint                       | 3.72E-02            | 1           | 6      | 84          | 6.15E+06 |
| α-terpinyl acetate| 80-26-2   | 17.73    | Wax                                    |                     |             | 8      | 80          | 1.66E+06 |
|                  |          |          |                                        |                     |             | 90     | 80          | 1.40E+06 |

S. Rice, J.A. Koziel / Data in Brief / S (2015) 553-706
| Compound                  | CAS Number | Boiling Point | Odor Notes                  |
|---------------------------|------------|---------------|-----------------------------|
| Terpinyl butyrate         | 2153-28-8  | 17.74         | Sour, Rosemary, Fruity,     |
|                           |            |               | Balsam                      |
| 2-ethyl-3,5-dimethylpyridine | 1123-96-2 | 17.91         |                             |
| +p-cresyl acetate         | 140-39-6   | 18.14         | Narcissus, Phenolic, Animal |
| m-tert-butylphenol        | 585-34-2   | 18.15         |                             |
| Verbenone                 | 80-57-9    | 18.16         | Camphor, Menthol, Celery    |
| 1-Tetradecanol            | 112-72-1   | 18.32         | Coconut                     |
| 3-methylhexane            | 589-34-4   | 18.32         |                             |
| +1-Tridecane              | 2437-56-1  | 18.33         |                             |
| 1-undecanol               | 112-42-5   | 18.34         | Mandarin, Waxy              |
| Octyl formate             | 112-32-3   | 18.34         | Fruity, rose, Orange, Waxy, |
| α-copaene                 | 3856-25-5  | 18.39         | Cucumber                    |
| α-cubebeene               | 17699-14-8 | 18.50         | Herb, Wax                   |
| (+)-sativene              | 3650-28-0  | 19.40         |                             |
| Nitro cyclohexane         | 1122-60-7  | 19.46         |                             |
| β-caryophyllene           | 87-44-5    | 19.66         | Wood, Spice, Spice          |
| +Benzyl alcohol           | 100-51-6   | 19.74         | Floral                      |
| Benzyl alcohol            | 100-51-6   | 19.74         | Floral                      |
| Compound | CAS      | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC  | OAV |
|----------|----------|----------|-----------------------|---------------------|-------------|--------|-------------|------|-----|
|          |          |          |                       |                     |             |        |             |      |     |
| Tyramine | 51-67-2  | 19.74    | Meaty                 |                     |             | A 7    | 96          | 5.83E+06 |     |
|          |          |          |                       |                     |             | B 1    | 13: 108 79 78 51 91 109 90 39 | 3.59E+06 |     |
|          |          |          |                       |                     |             | B 2    | 86 62 92 74 37 | 8.86E+05 |     |
|          |          |          |                       |                     |             | B 2    | 11: 108 107 77 80 76 106 49 |         |     |
| α-guaiene| 3691-12-1| 19.85    | Wood, Balsamic        |                     |             | A 5    | 6: 51 85 38 62 90 75 | 70     | 9.20E+06 |
|          |          |          |                       |                     |             | B 7    | 5: 90 62 109 37 61 | 70     | 3.71E+06 |
|          |          |          |                       |                     |             | B 1    | 1: 53       | 70     | 4.00E+06 |
|          |          |          |                       |                     |             | B 2    | 91 105 53 41 | 72     | 6.78E+05 |
|          |          |          |                       |                     |             | B 1    | 13: 108 107 77 80 76 106 49 |         |     |
|          |          |          |                       |                     |             | B 2    | 91 105 53 41 | 99     | 8.86E+05 |
| +Dimethylsulfone | 67-71-0  | 20.12    | Sulfur, Burnt         |                     |             | A 7    | 13: 109 71 28 39 | 91     | 4.00E+05 |
|          |          |          |                       |                     |             | B 4    | 13: 107 204 135 79 133 119 | 88     | 9.51E+04 |
| δ-cadinene| 483-76-1 | 20.20    | Thyme, Medicine, Wood |                     |             | A 7    | 105 147 81 148 73 65 95 | 80     | 1.93E+04 |
|          |          |          |                       |                     |             | B 3    | 2: 94 79   |         |     |
| 2,6-pyridinediamine | 141-86-6 | 20.49    | Wood                  |                     |             | A 5    | 19: 147 93 121 67 92 105 81 | 74     | 1.51E+04 |
|          |          |          |                       |                     |             | A 5    | 1: 109     | 71     | 4.03E+03 |
|          |          |          |                       |                     |             | A 1    | 19: 147 93 121 67 92 105 81 | 97     | 1.68E+06 |
|          |          |          |                       |                     |             | A 2    | 135 103 120 | 91     | 1.76E+05 |
|          |          |          |                       |                     |             | A 5    | 19: 147 93 121 67 92 105 81 | 98     | 3.99E+06 |
|          |          |          |                       |                     |             | A 6    | 189 106 82 204 95 | 96     | 1.75E+06 |
|          |          |          |                       |                     |             | A 7    | 19: 92 79 94 105 95 91 148 63 | 97     | 1.42E+06 |
|          |          |          |                       |                     |             | B 3    | 117         | 97     | 1.47E+06 |

S. Rice, J.A. Koziel / Data in Brief 5 (2015) 653–706
| Compound          | CAS Number | Retention Time (min) | Type  | Type  |
|-------------------|------------|----------------------|-------|-------|
| β-selinene        | 17066-67-0 | 21.25                | Herb  | Herb  |
| Longifolene       | 475-20-7   | 21.27                | Wood  |       |
| Alloaromadendrene | 25246-27-9 | 21.41                | Wood  | Wood  |
| α-bulnesene       | 3691-11-0  | 21.41                |       |       |
| α-gurjunene       | 489-40-7   | 21.43                | Wood  | Balsamic |
| Aromadendrene     | 489-39-4   | 21.48                | Wood  | Wood  |

| Peak | m/z | intensity | m/z | intensity |
|------|-----|-----------|-----|-----------|
| B 4  | 93  | 2.10E+05  | 1.75E+06 |
| 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 | 89 | 3.26E+05 |
| A 7  | 15: 161 162 134 94 190 43 91 | 72 | 1.56E+05 |
| 81 204 121 123 95 92 131 175 |       |           |
| B 3  | 92  | 1.84E+05  |       |           |
| B 4  | 85  | 4.15E+04  |       |           |
| A 1  | 20: 133 69 79 161 105 120 136 | 89 | 6.01E+06 |
| 81 77 106 119 162 121 39 109 94 175 92 82 123 |       |           |
| A 2  | 17: 189 106 92 41 148 190 81 | 89 | 2.39E+06 |
| 80 93 78 95 121 77 161 94 91 120 |       |           |
| A 5  | 17: 147 205 68 133 161 148 | 91 | 6.66E+05 |
| 189 105 175 93 107 135 109 123 53 69 134 |       |           |
| A 6  | 20: 41 133 93 69 107 147 148 | 90 | 4.19E+06 |
| 120 66 55 121 80 42 176 119 95 53 43 145 136 |       |           |
| A 7  | 87  | 1.16E+05  |       |           |
| B 3  | 90  | 3.11E+06  |       |           |
| B 4  | 105 135 69 43 42 109 | 89 | 1.96E+05 |
| 106 119 149 162 161 123 95 92 131 175 |       |           |
| A 6  | 20: 55 135 96 121 79 93 105 | 96 | 1.07E+06 |
| 161 148 106 204 120 91 80 127 94 77 122 205 104 |       |           |
| α-gurjunene       | 489-40-7   | 21.43                | Wood  | Balsamic |
| 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 81 | 81 | 1.34E+05 |
| 119 79 95 105 |       |           |
| B 3  | 81  | 5.86E+04  |       |           |
| B 4  | 81  | 3.10E+04  |       |           |
| Aromadendrene     | 489-39-4   | 21.48                | Wood  | Wood  |
| A 1  | 65  | 6.94E+04  |       |           |
| A 2  | 73  | 1.48E+05  |       |           |
| Compound                  | CAS     | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC | OAV |
|--------------------------|---------|----------|-----------------------|---------------------|-------------|--------|-------------|-----|-----|
| 2,4,6-trimethylpyridine  | 108-75-8| 21.66    |                       |                     |             | A 5    | 71          | 8.73E+04 |     |
| + Phenol                 | 108-95-2| 21.68    | Phenolic              | Phenolic            | 1.10E-01    | A 6    | 81          | 5.80E+04 |     |
| Dyclocaine               | 586-60-7| 21.69    |                       |                     |             | A 1    | 91          | 1.16E+05 |     |
| (-)-Aristolene           | 6831-16-9| 21.74   |                       |                     |             | A 7    | 87          | 9.66E+04 |     |
| +2-ethylphenol           | 90-00-6 | 21.91    | Phenolic              |                     |             | A 1    | 72          | 1.01E+04 |     |
| (+)-calarene             | 1734-55-3| 22.08   |                       |                     |             | A 5    | 70          | 6.94E+04 |     |
| α-cedrene                | 469-61-4| 22.08    | Woody, Cedar, Sweet, Fresh |               |             | A 2    | 71          | 2.89E+04 |     |
| Longicyclene             | 1137-12-8| 22.10  |                       |                     |             | A 5    | 78          | 6.42E+05 |     |
|                          |         |          |                       |                     |             | A 7    | 72          | 1.74E+04 |     |
|                          |         |          |                       |                     |             | A 5    | 78          | 1.57E+05 |     |
| Compound                        | CAS Number | Odor       |
|--------------------------------|------------|------------|
| γ-gurjunene                    | 22567-17-5 | Musty      |
| α-longipinene                  | 5989-08-2  | 22.18      |
| Cedryl acetate                 | 77-54-3    | Wood       |
| Valencene                      | 4630-07-3  | Green, Oil Citrus |
| 2-hydroxyethyl acrylate        | 5951-61-1  | 22.61      |
| Compound                                      | CAS         | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC | OAV          |
|----------------------------------------------|-------------|----------|-----------------------|---------------------|-------------|--------|-------------|-----|--------------|
| + Butylated Hydroxytoluene                   | 128-37-0    | 22.66    | Mild, Phenolic, Camphor|                     | B 4         |        |             |     | 7.39E+05     |
| Xylazine                                     | 7361-61-7   | 22.67    |                       |                     | B 1         | 84     |             |     | 3.39E+04     |
| 2,3,6-trimethylpyridine                      | 1462-84-6   | 23.95    |                       |                     | B 2         | 90     |             |     | 7.76E+04     |
| Toluene-2,4-diamine                          | 95-80-7     | 23.97    |                       |                     | A 2         | 66     |             |     | 7.76E+04     |
| Propofol                                     | 2078-54-8   | 23.97    | Phenolic              |                     | A 2         | 65     |             |     | 1.78E+04     |
| Butylated Hydroxytoluene and Xylazine        |             | 79       |                       |                     | A 2         | 4      |             |     | 7.76E+04     |
| 1-(3,6-Dimethyl-2-pyrazinyl)-2-methyl-1-propanone | 145984-66-3 | 23.98    |                       |                     | A 2         | 83     |             |     | 7.76E+04     |
| Methyl isoeugenol                            | 93-16-3     | 23.98    | Clove, Spice, Spice   |                     | A 2         | 121    |             |     | 1.50E+06     |
| Caryophyllene oxide                          | 1139-30-6   | 24.09    | Herb, Sweet, Spice    |                     | A 2         | 119    |             |     | 1.43E+05     |
| p-acetanisole                                | 100-06-1    | 24.58    | Anisic                |                     | A 2         | 117    |             |     | 2.69E+04     |
| 3-methyl-5-(1-methylethyl)-Phe- nol methylcarbamate| 2631-37-0 | 24.64    |                       |                     | A 2         | 115    |             |     | 1.43E+05     |
| Thymol                                       | 89-83-8     | 24.78    | Herbal                | 1.55E-02            | C 1         | 135    | 68         | 1.31E+04 |
| + Carvacrol                                  | 499-75-2    | 24.78    | Spicy                 | 1.12E-02            | C 1         | 135    | 70         | 1.31E+04 |
| 2,4-di-tert-butylphenol                     | 96-76-4     | 26.36    | Phenolic              |                     | A 4         | 191    | 68         | 2.90E+04 |
| α-bisabolol                                  | 72691-24-8  | 26.43    |                       |                     | A 5         | 207    | 77         | 3.95E+04 |
| Cyclobarbital                                | 52-31-3     | 35.80    |                       |                     | A 7         | 207    | 65         | 9.20E+03 |
| 1,4-Dioxane                                  | 123-91-1    | 38.37    |                       |                     | B 3         | 58     | 71         | 2.39E+03 |

If two references of ODTs are available, ODT from Devos, et al. [5] is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Section 1.5. 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. Underlined items highlight the compounds found in Pseudo Scent Marijuana. + Compounds indicate confirmation with reference standards, matching retention time and spectra.
Table 4
Summary of VOCs emitted from all illicit cocaine samples (sample code D in Section 1.5) and Sigma Pseudo™ Narcotic Scent Cocaine formulation (sample code E in Section 1.5) and sampled over 1 h at room temperature. Sigma Pseudo™ Narcotic Scent Cocaine formulation is indicated by underlined fonts.

| Compound               | CAS    | RT (min) | Published descriptors | Published ODT (ppm) | Sample 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 |
| +2-nitropropane        | 79-46-9| 1.11     |                       | 7.24E+00            | D 1         | 66     | 2.28E+06    | 2.68E+03 |
| 2,4-dimethylpentane    | 108-08-7| 1.16     |                       | 8.71E+01            | D 1         | 70     | 1.41E+05    | 1.62E+03 |
| 1,2-dimethyl hydrazine | 540-73-8| 1.18     |                       | 1.00E+01            | D 1         | 74     | 1.91E+04    |       |
| Ethyleimidine          | 151-56-4| 1.20     |                       |                    | D 2         | 68     | 7.08E+04    |       |
| Isobutane              | 75-28-5| 1.24     |                       |                    | D 3         | 85     | 3.13E+06    | 3.13E+05 |
| Ethyl Chloride         | 75-00-3| 1.26     |                       |                    | D 4         | 82     | 2.27E+05    | 2.27E+04 |
| +Butane                | 106-97-8| 1.26     |                       | 2.04E+02            | D 5         | 81     | 1.53E+05    | 1.53E+04 |
| Trichloromonofluoromethane | 75-69-4| 1.27     | Pungent, Ether        | Pungent, Ethereal, Aldehydic, Fruity | 1.50E-02  | 1.86E-01 | 5.39E+03    |       |
| +Acetaldehyde          | 75-07-0| 1.28     | Ethereal              | 4.35E+00            | D 2         | 77     | 5.39E+03    |       |
| +Ethyl ether           | 60-29-7| 1.31     | Ethereal              |                    | D 4         | 86     | 1.43E+04    |       |
| Isoprene               | 78-79-5| 1.33     | Ethereal              |                    | D 4         | 82     | 2.29E+04    |       |
| 4-methyldecane         | 2847-72-5| 1.39    | Ethereal              |                    | D 1         | 72     | 7.44E+04    |       |
|                        |        |          |                       |                    | D 2         | 65     | 5.04E+05    |       |
|                        |        |          |                       |                    | D 3         | 84     | 8.36E+05    |       |
|                        |        |          |                       |                    | D 4         | 65     | 2.98E+05    |       |
| Compound                  | CAS       | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models                | Net % match | PAC  | OAV   |
|--------------------------|-----------|----------|-----------------------|---------------------|-------------|-----------------------|-------------|------|-------|
|                          |           |          | Flavornet [7] TGSC [8]|                     | LRI & Odor  | Devos et al. [5]      |             |      |       |
| 2-methylpentane          | 107-83-5  | 1.39     |                       |                     |             |                       |             |      |       |
| 2,3-dimethylbutane       | 79-29-8   | 1.40     |                       |                     |             |                       |             |      |       |
| Hexane                   | 110-54-3  | 1.44     | Alkane                | 2.19E+01            |             |                       |             |      |       |
| Cyclopentane             | 287-92-3  | 1.45     | Petroleum             |                     |             |                       |             |      |       |
| 2-methylaziridine        | 75-55-8   | 1.45     |                       |                     |             |                       |             |      |       |
| 3-methylpentane          | 96-14-0   | 1.45     |                       |                     |             |                       |             |      |       |
| Isocyanatomethane        | 624-83-9  | 1.46     |                       |                     |             |                       |             |      |       |
| 2-hydroxy propanenitrile | 78-97-7   | 1.48     |                       |                     |             |                       |             |      |       |
| 3,4,5-trimethyl-1-hexene | 56728-10-0| 1.51     |                       |                     |             |                       |             |      |       |
| Compound                                  | CAS Number | Odor Description  | Relative Odor Concentration |
|-------------------------------------------|------------|--------------------|-----------------------------|
| Propanal                                  | 123-38-6   | Earthy, Alcohol, Wine, Whiskey, Cocoa, Nutty Sharp, Vinegar | 1.00E-02                    |
| Acetic anhydride                          | 108-24-7   | Pungent            | 5.89E-01                    |
| 2,2,4,4-tetramethyl-3-pentanone           | 815-24-7   | Sharp, Vinegar     | 5.89E-01                    |
| 2-methyl-2-propanamine                    | 75-64-9    | Pungent            | 1.00E-02                    |
| 2,2,4,4-tetramethyl-3-pentanone           | 815-24-7   | Pungent            | 5.89E-01                    |
| Acetone                                   | 67-64-1    | Solvent            | 1.45E+01                    |
| Methyl acetate                            | 79-20-9    | Ethereal           | 1.45E+01                    |
| Acrolein                                  | 107-02-8   | Almond, Cherry     | 1.74E-01                    |
| Propene                                   | 115-07-1   | Pungent            | 5.25E+01                    |
| Methacrylic anhydride                     | 760-93-0   | Spicy              | 4.07E-02                    |
| Isobutyraldehyde                          | 78-84-2    | Pungent, Malt, Green | 3.60E+03                  |
| 1-(ethenyloxy)-butane                     | 111-34-2   | Sweet, Musty, Alcoholic | 2.34E-01                  |
| 2,4-Pentanedione                          | 123-54-6   | Minty, Acetone     | 4.45E+05                    |
| Mefruside                                 | 7195-27-9  | Sweet, Musty       | 2.34E-01                    |
| Cyclohexane                               | 110-82-7   | Minty, Acetone     | 4.45E+05                    |
| 2,3,4-trimethylpentane                    | 565-75-3   | Sweet, Musty, Alcoholic | 2.34E-01                  |
| (S)-2-propylpiperidine                    | 458-88-8   | Sweet, Musty       | 2.34E-01                    |
| 2-ethyl-1-butanol                          | 97-95-0    | Sweet, Musty, Alcoholic | 2.34E-01                  |
| Nimorazole                                | 108-94-1   | Minty, Acetone     | 7.08E-01                    |
| 2,3,4-trimethylpentane                    | 565-75-3   | Minty, Acetone     | 7.08E-01                    |
| (S)-2-propylpiperidine                    | 458-88-8   | Sweet, Musty       | 2.34E-01                    |
| 2-ethyl-1-butanol                          | 97-95-0    | Sweet, Musty, Alcoholic | 2.34E-01                  |
| Nimorazole                                | 108-94-1   | Minty, Acetone     | 7.08E-01                    |
| 2,3,4-trimethylpentane                    | 565-75-3   | Minty, Acetone     | 7.08E-01                    |
| (S)-2-propylpiperidine                    | 458-88-8   | Sweet, Musty       | 2.34E-01                    |
| 2-ethyl-1-butanol                          | 97-95-0    | Sweet, Musty, Alcoholic | 2.34E-01                  |
| Nimorazole                                | 108-94-1   | Minty, Acetone     | 7.08E-01                    |

S. Rice, J.A. Koziel / Data in Brief 5 (2015) 653–706
| Compound | CAS      | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC | OAV |
|----------|----------|----------|-----------------------|---------------------|-------------|--------|-------------|-----|-----|
| 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 |                     | 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                  |                     | D 4         | 3: 100 57 41 | 67     | 1.24E+04 |     |
| 1,2-diethyl hydrazine | 1615-80-1 | 2.31     | Mint                  |                     | D 4         | 6: 88 70 89 73 87 60 | 73     | 5.77E+05 |     |
| + Ethylacetate | 141-78-6 | 2.31     | Pineapple             | Ethereal, Fruity, Sweet, Weedy, Green | D 1         | 9: 43 61 70 73 62 71 60 89 55 | 99     | 3.08E+06 1.17E+06 |     |
| + 2-methyl-3-pentanone | 565-69-5 | 2.22     | Mint                  |                     | D 3         | 6: 61 70 73 62 90 60 | 71     | 4.00E+06 1.52E+06 |     |
| + Heptane | 142-82-5 | 2.22     | Alkane, Sweet, Ethereal |                     | D 3         | 10: 43 61 42 70 88 45 73 62 | 99     | 3.29E+06 1.25E+06 |     |
| + 2-methyl-3-pentanone | 565-69-5 | 2.22     | Mint                  |                     | D 4         | 7: 70 88 73 42 74 62 59 | 71     | 2.31E+06 8.80E+05 |     |
| + Ethylacetate | 141-78-6 | 2.31     | Pineapple             | Ethereal, Fruity, Camphor | D 5         | 7: 70 88 73 42 74 62 59 | 71     | 2.31E+06 8.80E+05 |     |
| Methyl thiocyanate | 556-64-9 | 2.33     | Sulfur                | Sulfury, Onion      | D 5         | 4: 42 73 46 60 | 66     | 3.15E+05 2.03E+06 |     |
| + Ethanol | 64-17-5 | 2.34     | Sweet                 | Alcoholic           | D 2         | 1: 45 | 87     | 4.09E+05 1.42E+04 |     |
| + Isopropyl alcohol | 67-63-0 | 2.34     | Alcohol, Musty, Woody |                     | D 2         | 1: 45 | 81     | 2.69E+05 2.63E+04 |     |
| + Formic acid | 64-18-6 | 2.34     | Acetic                |                     | D 4         | 1: 45 | 80     | 5.72E+05 5.59E+04 |     |
| Nitrogen dioxide | 10102-44-0 | 2.34 | Acetic                |                     | D 4         | 1: 45 | 79     | 5.72E+05 5.59E+04 |     |
| methylhydrazine | 60-34-4 | 2.35     |                      |                     | D 5         | 1: 46 | 78     | 1.95E+05 9.05E+04 |     |
| Acetic acid ethenyl ester | 108-05-4 | 2.41     |                      |                     | D 5         | 1: 46 | 76     | 6.16E+03 3.31E+04 |     |
| + Methylen chloride | 75-09-2 | 2.41     |                      |                     | D 5         | 1: 46 | 76     | 6.16E+03 3.31E+04 |     |
| Tolycaine | 3686-58-6 | 2.43     | Ether, Fruit          | Sweet, Fruity, Ethereal, Wine, Banana, Woody | D 5         | 4: 86 49 84 43 | 72     | 6.97E+04 4.50E+04 |     |
| + 2-Pentanone | 107-87-9 | 2.43     | Ether, Fruit          | Sweet, Fruity, Ethereal, Wine, Banana, Woody | 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 |     |
| Chemical Name | CAS Number | Molecular Weight | Notes                                                                 |
|---------------|------------|------------------|----------------------------------------------------------------------|
| Methyl cyclohexane | 108-87-2 | 106.18 | 2.61 D 3 5: 83 56 41 69 39 94 1.24E +05 |
| +n-Propyl acetate | 109-60-4 | 106.17 | 2.68 D 3 5: 98 55 82 85 75 4.99E +06 |
| +1-Heptanol | 111-70-6 | 118.19 | 2.77 D 3 7: 70 88 73 42 74 62 59 2.31E +06 |
| Ethanedinitrile | 460-19-5 | 74.08 | 3.00 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| Benzene | 71-43-2 | 78.11 | Aromatic 3.63E +00 D 1 93 1.32E +05 |
| 2,5-dimethyl hexane | 592-13-2 | 90.19 | 3.17 D 3 6: 70 53 43 39 99 56 9.76E +05 |
| 3-methylheptane | 589-81-1 | 90.19 | 3.35 D 3 6: 70 53 43 39 99 56 9.76E +05 |
| Sorbic Acid | 110-44-1 | 124.02 | 1.29E +05 |
| +Isothiocyanato methane | 556-61-6 | 126.07 | 3.76 D 3 7: 70 88 73 42 74 62 59 2.31E +06 |
| Chloroform | 67-66-3 | 94.02 | 3.77 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| Ethylenediamine | 107-15-3 | 60.13 | 3.93 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| +1,1-dimethyl-hydrazine | 57-14-7 | 64.10 | 3.95 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| 3-pentanol | 584-02-1 | 72.13 | 3.95 Fruit D 3 5: 83 69 82 55 39 94 1.24E +05 |
| Hydrazine | 302-01-2 | 40.05 | 3.96 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| +Octane | 111-65-9 | 86.15 | 4.00 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| Tetrahydrofurfuryl acetate | 637-64-9 | 110.20 | 4.07 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| Isobutyl acetate | 110-19-0 | 100.19 | 4.86 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| +Isobutyric acid | 79-31-2 | 88.19 | 4.88 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| +Toluene | 108-88-3 | 92.19 | 5.05 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| +Phenylethyl alcohol | 60-12-8 | 106.19 | 5.05 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| +1-butanol | 71-36-3 | 74.19 | 6.15 D 3 5: 83 69 82 55 39 94 1.24E +05 |
| +Isobutanol | 78-83-1 | 88.19 | 6.17 D 3 5: 83 69 82 55 39 94 1.24E +05 |

S. Rice, J.A. Koziel / Data in Brief 5 (2015) 653–706
| Compound                          | CAS     | RT (min) | Published descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC     | OAV     |
|----------------------------------|---------|----------|-----------------------|---------------------|-------------|--------|-------------|---------|---------|
| Propanoic acid, anhydride        | 123-62-6| 6.49     |                       |                     |             | LRI & Odor [6] Devos et al. [5] |  |  |  |
| 4-methyl-3-penten-2-one          | 141-79-7| 6.65     | Sweet, Chemical       |                     | D 3 1: 57    |  |  |        |         |
| +Decane                          | 124-18-5| 6.66     | Alkane                |                     | D 3 1: 57    |  |  |        |         |
| +Isoamyl alcohol                 | 123-51-3| 7.52     | Whiskey, Malt, Burnt Balsamic |                 | D 4 3: 55 70 53 |  |  |        |         |
| Amyl alcohol                     | 71-41-0 | 7.54     | Fusel oil, Alcoholic, Whiskey, Fruity, Banana |   | D 1 79 2.43E+04 5.45E+05 |  |  |        |         |
| 4-p-xylene                       | 106-42-3| 7.65     | Pine, Turpentine, Turpentine, Terpenic |           | D 3 2: 91 105 |  |  |        |         |
| a-pinene                         | 80-56-8 | 7.90     | Parfum, Turpentine, Mint, Spice Camphor |     | D 1 79 1.18E+04 1.70E+04 |  |  |        |         |
| a-phellandrene                   | 99-83-2 | 7.91     | Pine, Terpentine, Terpentine, Woody |         | D 1 79 1.18E+04 |  |  |        |         |
| +Camphene                        | 79-92-5 | 10.21    | Sweet, Camphor       |                     | D 3 5: 120 105 91 155 136 |  |  |        |         |
| p-ethyltoluene                   | 622-96-8| 10.25    | Sweet, Camphor       |                     | D 3 4: 105 154 77 91 |  |  |        |         |
| 2-ethyltoluene                   | 611-14-3| 10.61    | Sweet, Camphor       |                     | D 3 7: 57 70 112 83 69 72 155 |  |  |        |         |
| 2,2,5-trimethylhexane            | 3522-94-9| 10.67    | Resin, Flower, Green |                     | D 5 2: 91 105 |  |  |        |         |
| 1-hexanol                        | 111-27-3| 10.73    | Resin, Flower, Green |                     | D 5 2: 91 105 |  |  |        |         |
| Diacetone alcohol                | 123-42-2| 10.79    |                       |                     | D 3 1: 57    |  |  |        |         |
| 1,3,5-trimethylbenzene           | 108-67-8| 11.02    |                       |                     | D 5 2: 91 105 |  |  |        |         |
| +Piperidine                      | 110-89-4| 11.20    |                       |                     | D 3 2: 91 105 |  |  |        |         |
| 2,4,5-trimethylbenzenamine       | 137-17-7| 11.30    |                       |                     | D 3 1: 57    |  |  |        |         |
| Compound               | CAS      | RT  (min) | Published descriptors | Published descriptors | Published descriptors | Published ODT (ppm) | Sample code | Models       | Net % match | PAC       | OAV       |
|------------------------|----------|-----------|-----------------------|-----------------------|-----------------------|---------------------|-------------|--------------|-------------|-----------|-----------|
|                        |          |           |                       |                       |                       |                     |             | LRI & Odor  |             |           |           |
|                        |          |           |                       |                       |                       |                     |             | Devos et al. [5]|             |           |           |
| Indane                 | 496-11-7 | 14.10     |                       |                       |                       |                     |             |              |             |           |           |
| Isobutyrophenone       | 611-70-1 | 14.10     |                       |                       |                       |                     |             |              |             |           |           |
| + Nonane               | 111-84-2 | 14.13     | Alkane                | Gasoline              |                       | 1.26E+00            | D 3          |              |             |           |           |
| 2-chloroacetophenone   | 532-27-4 | 14.14     |                       |                       |                       | 2.57E-02            | D 1          |              |             |           |           |
| + Undecane             | 1120-21-4| 14.14     | Alkane                |                       |                       | 1.17E+00            | D 3          |              |             |           |           |
| 2,2-dimethylbutane     | 75-83-2  | 14.15     |                       |                       |                       |                     |             |              |             |           |           |
| + Dodecane             | 112-40-3 | 14.15     | Alkane                | Alkane                |                       | 2.04E+00            | D 5          |              |             |           |           |
| + Tridecane            | 629-50-5 | 14.17     | Alkane                | Alkane                |                       | 2.14E+00            | D 1          |              |             |           |           |
| Octyl acetate          | 112-14-1 | 14.20     |                       |                       |                       | 3.98E-03            | D 1          |              |             |           |           |
| N-Nitrosodimethylamine | 62-75-9  | 14.66     |                       |                       |                       |                     |             |              |             |           |           |
| + 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 |
| Hydroxyethylhydrazine  | 109-84-2 | 14.91     | Fruit                 |                       |                       |                     |             |              |             |           |           |
| + 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 87 | 168 | 9.77E+04 | 9.77E+04 |
| tetrahydro-2-methyl-2- furanol | 7326-46-7 | 15.59     |                       |                       |                       |                     |             |              |             |           |           |
| + 1-methyl-1H-pyrrole  | 96-54-8  | 15.72     |                       |                       |                       |                     |             |              |             |           |           |
| 2-ethoxyethanol        | 110-80-5 | 15.79     |                       |                       |                       |                     |             |              |             |           |           |
| Compound                        | CAS No. | RT    | Detection Threshold | Code | OAV   |
|--------------------------------|---------|-------|---------------------|------|-------|
| Hexestrol                      | 84-16-2 | 15.85 | D 1                 | 73   | 8.19E+04 |
| Methyl benzoate                | 93-58-3 | 16.30 | Prune, Lettuce, Herb, Sweet | 1.07E-01 | D 1 | 11: 105 77 136 76 137 106 39 99 1.81E+06 1.69E+07 |
| Cumene                         | 98-82-8 | 16.49 | Phenolic            | 2.40E-02 | D 3 | 5: 105 135 120 77 78 77 2.84E+05 1.18E+07 |
| +Acetophenone                  | 98-86-2 | 16.49 | Floral              | 6.50E-02 | D 3 | 5: 105 135 120 77 78 93 2.84E+05 7.81E+05 |
| 3-ethyltoluene                 | 620-14-4 | 16.50 | Fruit, Sweet, Herb, Sweet | 4.90E-02 | D 3 | 4: 78 105 120 106 78 1.52E+05 |
| 2,2,4-trimethylpentane         | 540-84-1 | 16.53 | Coffee bean, Nutty | 3.63E-01 | D 3 | 4: 56 57 55 43 66 8.44E+04 |
| 2-ethyl-5-methylpyrazine       | 13360-64-0 | 16.81 | Fruit, Sweet, Herb, Sweet | 5.07E-02 | D 3 | 3: 121 122 81 73 3.39E+04 |
| γ-hexalactone                  | 695-06-7 | 17.20 | Coffee bean, Nutty | 5.65E-02 | D 3 | 4: 56 85 69 51 68 2.89E+05 |
| 2-ethyl-3,5-dimethylpyridine   | 1123-96-2 | 17.90 | Mild, Green, Sweet, Earthy | 1.80E+05 | D 3 | 6: 122 105 78 77 136 102 89 1.71E+05 |
| +α-α-Dimethylbenzenemethanol   | 617-94-7 | 18.05 | Sweet, Fruity, Spicy, Anisic, Balsam | 8.76E-02 | D 3 | 7: 43 70 41 56 39 42 100 70 4.60E+03 |
| p-methoxyphenylacetone         | 122-84-9 | 18.07 | Sweet, Fruity, Spicy, Anisic, Balsam | 8.76E-02 | D 3 | 5: 198 140 154 82 100 98 3.83E+06 |
| 3-methylhexane                 | 589-34-4 | 18.33 | Alkane              | 6.76E-02 | D 3 | 4: 111 83 97 106 74 2.87E+04 4.24E+05 |
| +Tetradecane                   | 629-59-4 | 18.34 | Alkane              | 6.76E-02 | D 3 | 5: 83 56 41 69 39 74 2.15E+05 |
| 1-undecanol                    | 112-42-5 | 18.37 | Waxy                | 6.76E-02 | D 3 | 5: 198 140 154 82 100 98 3.83E+06 |
| Nitrocyclohexane               | 1122-60-7 | 19.50 | Alkane              | 6.76E-02 | D 3 | 5: 182 112 154 82 100 98 3.83E+06 |
| β-caryophyllene                | 87-44-5 | 19.68 | Wood, Spice         | 6.40E-02 | D 3 | 6: 122 105 78 77 136 102 89 1.71E+05 |
| +Pentadecane                   | 629-62-9 | 20.28 | Alkane              | 6.76E-02 | D 3 | 8: 41 56 57 86 85 99 112 70 86 1.74E+05 |
| +Butanoic acid, butyl ester    | 109-21-7 | 20.97 | Alkane              | 6.76E-02 | D 3 | 8: 41 56 57 86 85 99 112 70 86 1.74E+05 |
| Longifolene                    | 475-20-7 | 21.28 | Waxy                | 6.76E-02 | D 3 | 8: 41 56 57 86 85 99 112 70 86 1.74E+05 |
| Toluene-2,4-diamine            | 95-80-7 | 23.91 | Alkane              | 6.76E-02 | D 3 | 8: 41 56 57 86 85 99 112 70 86 1.74E+05 |
| 2,3,6-trimethylpyridine        | 1462-84-6 | 23.96 | Alkane              | 6.76E-02 | D 3 | 8: 41 56 57 86 85 99 112 70 86 1.74E+05 |

If two references for ODTs are available, ODT from Devos, et al. [5] is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Section 1.5. 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. Underlined items highlight the compounds found in Pseudo Scent Cocaine. + Compounds indicate confirmation with reference standards, matching retention time and spectra.
Table 5
Summary of VOCs emitted from all illicit heroin samples (sample code F in Section 1.5) and Sigma Pseudo™ Narcotic Scent Heroin formulation (sample code G in Section 1.5) and sampled over 1 h at room temperature. Sigma Pseudo™ Narcotic Scent Heroin formulation is indicated by underlined fonts.

| Compound                  | CAS       | RT (min) | Published Descriptors | Published ODT (ppm) | Sample 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 |
| +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     | Wine, Solvent,        |                     | F 1         | 2: 50 52   | 73  | 1.00E+04 |
| +Isobutanol               | 78-83-1   | 1.19     | Ethereal, Winey       |                     | F 1         | 2: 50 52   | 70  | 4.81E+04 |
| Hexane                    | 110-54-3  | 1.19     | Alkane                | 2.19E+01            | F 1         | 6: 43 57 41 56 39 | 68  | 7.74E+04 3.54E+03 |
| Isobutane                 | 75-28-5   | 1.23     |                       | 1.00E+01            | F 1         | 10: 43 42 57 72 39 55 56 83 | 8.96E+05 8.96E+04 |
| Isobutyraldehyde          | 78-84-2   | 1.23     | Pungent, Malt,        | 4.07E-02            | F 1         | 10: 43 42 57 72 39 55 56 83 | 8.96E+05 2.20E+07 |
| 4-methyldecane            | 2847-72-5 | 1.39     |                       |                     | F 1         | 3: 43 41 42 | 67  | 4.33E+05 |
| 2-methylpentane           | 107-83-5  | 1.39     |                       | 4.25E+01            | F 2         | 3: 42 39 41 | 66  | 4.19E+05 |
| Ethylenimine              | 151-56-4  | 1.40     |                       |                     | F 1         | 3: 43 42 41 | 66  | 4.33E+05 |
| 2,3-dimethylbutane        | 79-29-8   | 1.40     |                       |                     | F 1         | 3: 43 42 41 | 66  | 4.33E+05 |
| 3,4,5-trimethyl-1-hexene  | 56728-10-0| 1.40     |                       |                     | F 1         | 3: 43 42 41 | 66  | 4.33E+05 |
| 3-methylhexane            | 589-34-4  | 1.40     |                       |                     | F 2         | 3: 43 42 41 | 66  | 4.33E+05 |
| +1-butanol                | 71-36-3   | 1.42     | Medicine, Fruit,      | 4.90E-01            | F 1         | 3: 43 42 41 57 52 39 | 66  | 7.94E-04 1.58E+05 |
| 3-methylpentane           | 96-14-0   | 1.45     |                       |                     | F 1         | 3: 43 42 41 | 66  | 4.33E+05 |
| 2-methylaziridine         | 75-55-8   | 1.49     |                       | 4.25E+01            | F 2         | 3: 42 39 41 | 66  | 4.19E+05 |
| Isocyanatomethane         | 624-83-9  | 1.52     | Solvent               | 5.25E+01            | F 2         | 3: 42 39 41 | 73  | 3.41E+04 6.50E+02 |
| Tolycaine                 | 3686-58-6 | 1.52     | Solvent               | 2.04E+02            | F 1         | 4: 58 45 42 38 | 74  | 1.45E+05 7.10E+02 |
| +Propene                  | 115-07-1  | 1.65     |                       |                     | F 1         | 4: 58 45 42 38 | 79  | 2.36E+05 1.15E+03 |
| +Butane                   | 106-97-8  | 1.66     |                       |                     | F 2         | 4: 58 45 42 38 | 92  | 1.45E+05 1.00E+04 |

S. Rice, J.A. Kozel / Data in Brief 5 (2015) 653–706
| Chemical Name          | CAS Number | Mol. Wt. | Odor Descriptions                                      | F 1 | F 2 |
|-----------------------|------------|---------|--------------------------------------------------------|-----|-----|
| Hydrazine             | 302-01-2   | 43     | 3.00E+00, 1.97                                        | F 2 | 5: 43 58 39 37 38 97 | 3.14E+05 2.18E+04 |
| Cyclohexane           | 110-82-7   | 1.98   | 2.19E+01 G 1: 39 84 56 42 55 69 85 50 54             | F 1 | 1: 33 78 | 1.19E+03 3.97E+02 |
| + Ethylacetate        | 141-78-6   | 2.32   | Pineapple Ethereal, Fruity, Sweet, Weedy, Green       | F 2 | 96 | 2.71E+05 1.24E+04 |
| Propylene glycol      | 57-55-6    | 2.33   | 2.63E+00                                            | F 2 | 96 | 2.41E+05 5.17E+04 |
| + Isopropyl alcohol   | 67-63-0    | 2.33   | Alcohol, Musty, Woody                                | F 2 | 65 | 8.74E+04 |
| + Ethanol             | 64-17-5    | 3.66   | 2.88E+01 F 2: 3 45 61 44                              | F 2 | 68 | 6.90E+04 2.39E+03 |
| + Acetic anhydride    | 108-24-7   |        | 5.89E-01 F 2: 2 43 42                                | F 2 | 76 | 6.24E+03 1.06E+04 |
| nitrocyclohexane      | 1122-60-7  | 10.29  | G 1 1: 43                                            | G 2 | 69 | 3.64E+04 6.18E+04 |
| m-cymene              | 535-77-3   | 11.33  | G 1 3: 83 55 41                                    | G 1 | 74 | 2.39E+04 |
| 1-(3-methylphenyl)-   | 585-74-0   | 11.34  | G 1 1: 43                                            | G 1 | 93 | 4.08E+04 |
| tert-butyl-benzene    | 98-06-6    | 11.34  | G 1 1: 43                                            | G 1 | 86 | 2.84E+04 |
| 1,2,3,4-tetramethylbenzene | 488-23-3 | 11.35  | G 1 1: 43                                            | G 1 | 88 | 2.84E+04 |
| + p-cymene            | 99-87-6    | 11.35  | 2.63E-02 F 1: 3 120 119 134                          | F 1 | 66 | 2.94E+04 1.12E+06 |
| Isodurene             | 527-53-7   | 11.37  | 1.45E-01 F 2: 5 43 60 41 59 47                        | F 2 | 97 | 5.74E+07 3.97E+08 |
| Nitrogen dioxide      | 10102-44-0 | 12.29  | 1.86E-01 G 1: 1: 46                                 | G 1 | 76 | 9.21E+02 4.95E+03 |
| + Furfural            | 98-01-1    | 12.71  | 7.76E-01 F 2: 3 120 119 134                         | F 2 | 93 | 3.22E+04 4.15E+04 |
| Fenbendazole          | 43210-67-9 | 12.98  | 3.55E-02 F 1: 3 267 269 268                         | F 1 | 66 | 5.95E+04 |
| + Propanoic acid      | 79-09-4    | 13.91  | 5.40E-02 F 2: 105 77 105                             | G 1 | 76 | 5.40E+04 1.30E+06 |
| Propanoic acid,       | 123-62-6   | 13.91  | 4.79E-03 F 2: 5 57 209 193 82 69                      | F 2 | 68 | 3.17E+03 |
| anhydride             | 100-52-7   | 14.10  | 3.00E-03 F 2: 105 77                                  | G 1 | 66 | 4.74E+03 |
| Benzaldehyde          | 352-27-4   | 14.10  | 2.57E-02 G 1: 1 267 268                               | G 1 | 77 | 5.40E+04 2.10E+06 |
| + 2-chloroacetophenone| 611-70-1   | 14.10  | Green                                                  | G 1 | 66 | 3.06E+04 |
| Ethyl cyclohexane     | 1678-91-7  | 15.20  | G 1 1: 83                                            | G 1 | 70 | 7.33E+04 |
| Butyric acid          | 107-92-6   | 15.53  | 3.89E-03 F 1: 3 60 42 37                              | F 1 | 95 | 4.20E+05 1.08E+08 |
| + Pentanoic acid      | 109-52-4   | 15.53  | 4.79E-03 F 1: 5 60 45 73 43 39                        | F 1 | 89 | 3.45E+05 7.22E+07 |
| 2,2-dimethylbutane    | 75-83-2    | 15.87  | 1.07E-01 G 1: 2                                        | G 1 | 97 | 1.74E+05 1.63E+06 |
| Methyl benzoate       | 93-58-3    | 16.26  | 1.55E+00 F 2: 80                                       | F 2 | 80 | 2.84E+04 1.84E+04 |
| + Toluene             | 108-88-3   | 19.16  |                                                          |     |    |
| Compound          | CAS    | RT (min) | Published Descriptors | Published ODT (ppm) | Sample code | Models | Net % match | PAC     | OAV     |
|------------------|--------|----------|-----------------------|--------------------|-------------|--------|-------------|---------|---------|
| +Dimethylsulfone | 67-71-0| 20.11    | Sulfur, Burnt         | TGSC [8]           | Devos et al. [5] | F 2    | 2: 79 62    | 96      | 1.9E+05 |
| Methyl formate   | 107-31-3| 22.87    | Sulfurous, Burnt      | 9.33E+01           | 60          | 1: 60  | 73          | 1.83E+03| 1.96E+01|
| Diethyl Phthalate| 84-66-2| 27.46    | Fruity, Plum          | 9.71E+03           |             |        |             |         |         |

If two references for ODTs are available, ODT from Devos, et al. [5] is used to calculate OAV. RT = Retention Time. ODT = Odor Detection Threshold. Code, see Section 1.5. 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. Underlined items highlight the compounds found in Pseudo Scent Heroin. + Compounds indicate confirmation with reference standards, matching retention time and spectra.
| Compound                  | CAS      | Sample code | Rank conc. | Rank OAV | Change in ranking |
|--------------------------|----------|-------------|------------|----------|------------------|
| Limonene                 | 138-86-3 | A 1         | 1          | 1        | –4               |
| Limonene                 | 138-86-3 | A 2         | 2          | 2        | –5               |
| Isobutane                | 75-28-5  | A 3         | 3          | 3        | –5               |
| Ethylene oxide           | 75-21-8  | A 4         | 4          | 4        | –16              |
| (±)-sativene             | 3650-28-0| A 5         | 5          | 5        | No ODT           |
| Acetic acid              | 64-19-7  | A 6         | 6          | 1        | –1               |
| Benzylic alcohol         | 100-51-6 | A 7         | 1          | 1        | No ODT           |
| Tyramine                 | 51-67-2  | B 1         | 1          | 1        | No ODT           |
| β-pinene                 | 18172-67-3| B 2        | 1          | 1        | No ODT           |
| Acetic acid              | 64-19-7  | B 3         | 1          | 1        | –1               |
| Butyl formate            | 592-84-7 | B 4         | 1          | 1        | No ODT           |
| γ-terpinene              | 99-85-4  | C 1         | 1          | 1        | No ODT           |
| γ-terpinene              | 99-85-4  | C 2         | 1          | 1        | No ODT           |
| Camphene                 | 79-92-5  | C 3         | 1          | 1        | No ODT           |
| Camphene                 | 79-92-5  | A 1         | 1          | 2        | No ODT           |
| Camphene                 | 79-92-5  | A 2         | 2          | 2        | No ODT           |
| 2-methylpentane          | 107-83-5 | A 3         | 2          | 2        | No ODT           |
| Acetone                  | 67-64-1  | A 4         | 2          | 1        | 12               |
| Benzylic alcohol         | 100-51-6 | A 5         | 2          | 1        | No ODT           |
| Methylisohexenyl ketone  | 110-93-0 | A 6         | 2          | 3        | –1               |
| Acetone                  | 67-64-1  | A 7         | 2          | 21       | –19              |
| β-pinene                 | 18172-67-3| B 1        | 1          | 1        | No ODT           |
| Myrcene                  | 123-35-3 | B 2         | 2          | 1        | +1               |
| Methylisohexenyl ketone  | 110-93-0 | B 3         | 2          | 3        | –1               |
| Acetone                  | 67-64-1  | B 4         | 2          | 2        | 14               |
| Ethyl benzene            | 100-41-4 | C 1         | 2          | 2        | –1               |
| Terpinolene              | 586-62-9 | C 2         | 2          | 3        | –1               |
| γ-terpinene              | 99-85-4  | C 3         | 2          | 2        | No ODT           |
| Isobornyl thiocyanacetate| 115-31-1 | A 1         | 3          | 3        | No ODT           |
| Isobornyl thiocyanacetate| 115-31-1 | A 2         | 3          | 3        | No ODT           |
| 3,4,5-trimethyl-1-hexene | 56728-10-0| A 3        | 3          | 3        | No ODT           |
| Limonene                 | 138-86-3 | A 4         | 3          | 4        | –1               |
| Tyramine                 | 51-67-2  | A 5         | 3          | 3        | No ODT           |
| β-caryophyllene          | 87-44-5  | A 6         | 3          | 4        | –1               |
| Tyramine                 | 51-67-2  | A 7         | 3          | 3        | No ODT           |
| Myrcene                  | 123-35-3 | B 1         | 3          | 3        | +2               |
| Limonene                 | 138-86-3 | B 2         | 3          | 4        | –1               |
| β-caryophyllene          | 87-44-5  | B 3         | 3          | 4        | –1               |
| 3-pentanol               | 584-02-1 | B 4         | 3          | 5        | –2               |
| m-cymene                 | 535-77-3 | C 1         | 3          | 3        | No ODT           |
| Ethyl benzene            | 100-41-4 | C 2         | 3          | 5        | –2               |
| Terpinolene              | 586-62-9 | C 3         | 3          | 3        | 0                |
| β-pinene                 | 18172-67-3| A 1        | 4          | 4        | No ODT           |
| Isobutane                | 75-28-5  | A 2         | 4          | 13       | –9               |
| 4-methyldecane           | 2847-72-5| A 3         | 4          | 4        | No ODT           |
| Camphene                 | 79-92-5  | A 4         | 4          | 4        | No ODT           |
| Isobutane                | 75-28-5  | A 5         | 4          | 9        | No ODT           |
| Longifolene              | 475-20-7 | A 6         | 4          | 4        | No ODT           |
| Isobutane                | 75-28-5  | A 7         | 4          | 22       | –18              |
| Ethylene oxide           | 75-21-8  | B 1         | 4          | 28       | –24              |
| Camphene                 | 79-92-5  | B 2         | 4          | 2        | No ODT           |
| Longifolene              | 475-20-7 | B 3         | 4          | 4        | No ODT           |
| tert-butanol             | 75-65-0  | B 4         | 4          | 4        | No ODT           |
| p-cymene                 | 99-87-6  | C 1         | 4          | 1        | +3               |
| m-cymene                 | 535-77-3 | C 2         | 4          | 4        | No ODT           |
| m-cymene                 | 535-77-3 | C 3         | 4          | 4        | No ODT           |
| Isobutane                | 75-28-5  | A 1         | 5          | 11       | –6               |
| Isobutylaldehyde         | 78-84-2  | A 2         | 5          | 3        | +2               |
| Compound                      | CAS       | Sample code | Rank conc. | Rank OAV | Change in ranking |
|-------------------------------|-----------|-------------|------------|----------|-------------------|
| Ethylene oxide               | 75-21-8   | A 3         | 5          | 19       | –14               |
| 2,2,4-trimethylpentane       | 540-84-1  | A 4         | 5          | No ODT   |                   |
| γ-gurjunene                  | 22567-17-5| A 5         | 5          | No ODT   |                   |
| **Acetone**                  | **67-64-1**| A 6         | 5          | **22**   | –17               |
| Butane                       | **106-97-8**| A 7         | 5          | **34**   | –29               |
| Benzyl alcohol               | 100-51-6  | B 1         | 5          | No ODT   |                   |
| α-phellandrene               | 99-83-2   | B 2         | 5          | No ODT   |                   |
| Fenchyl alcohol              | 1632-73-1 | B 3         | 5          | No ODT   |                   |
| Propylene oxide              | 107-10-8  | B 4         | 5          | 1        | +4                |
| 1,2,3,4-tetramethylbenzene   | 488-23-3  | C 1         | 5          | 2        | +3                |
| p-cymene                     | 99-87-6   | C 2         | 5          | 1        | +4                |
| p-cymene                     | 99-87-6   | C 3         | 5          | 1        | +4                |
| Isobutyraldehyde             | 78-84-2   | A 1         | 6          | 1        | +5                |
| β-pinene                     | 18172-67-3| A 2         | 6          | No ODT   |                   |
| Limonene                     | 138-86-3  | A 3         | 6          | 4        | +2                |
| Methylene chloride           | 75-09-2   | A 4         | 6          | 15       | –9                |
| α-humulene                   | 6753-98-6 | A 5         | 6          | 17       | –11               |
| **Butane**                   | **106-97-8**| A 6         | 6          | **31**   | –25               |
| α-phellandrene               | 99-83-2   | A 7         | 6          | No ODT   |                   |
| Butane                       | 106-97-8  | B 1         | 6          | 25       | –19               |
| α-pinene                     | 80-56-8   | B 2         | 6          | 5        | +1                |
| Butane                       | 106-97-8  | B 3         | 6          | 35       | –29               |
| Ethylene oxide               | 75-21-8   | B 4         | 6          | 23       | –17               |
| 1-ethyl-3,5-dimethylbenzene  | 934-74-7  | C 1         | 6          | No ODT   |                   |
| 1,2,3,4-tetramethylbenzene   | 488-23-3  | C 2         | 6          | 2        | +4                |
| 1,2,3,4-tetramethylbenzene   | 488-23-3  | C 3         | 6          | 2        | +4                |
| Betahisine                   | 5638-76-6 | A 1         | 7          | No ODT   |                   |
| α-pinene                     | 80-56-8   | A 2         | 7          | 10       | –3                |
| Camphene                     | 79-92-5   | A 3         | 7          | No ODT   |                   |
| Methylisohexenyl ketone      | 110-93-0  | A 4         | 7          | 2        | +5                |
| Valencene                    | 4630-07-3 | A 5         | 7          | No ODT   |                   |
| **Fenchyl alcohol**          | **1632-73-1**| A 6         | 7          | No ODT   |                   |
| δ-3-carene                   | **13466-78-9**| A 7         | 7          | **20**   | –13               |
| Acetone                      | 67-64-1   | B 1         | 7          | 17       | –10               |
| Benzyl alcohol               | 100-51-6  | B 2         | 7          | No ODT   |                   |
| Acetone                      | 67-64-1   | B 3         | 7          | 31       | –24               |
| Diacetone alcohol            | 123-42-2  | B 4         | 7          | 10       | –3                |
| Isodurene                    | 527-53-7  | C 1         | 7          | No ODT   |                   |
| 2-acetyl-6-methyl pyrazine   | 22047-26-3| C 2         | 7          | No ODT   |                   |
| 2-Butanol                    | 78-92-2   | C 3         | 7          | 4        | +3                |
| α-phellandrene               | 99-83-2   | A 1         | 8          | No ODT   |                   |
| Terpinolene                  | 586-62-9  | A 2         | 8          | 8        | 0                 |
| Isobutyraldehyde             | 78-84-2   | A 3         | 8          | 2        | +6                |
| 2-butane                     | 78-93-3   | A 4         | 8          | 13       | –5                |
| 3,4,5-trimethyl-1-hexene     | 56728-10-0| A 5         | 8          | No ODT   |                   |
| α-humulene                   | **6753-98-6**| A 6         | 8          | **8**    | 0                 |
| α-humulene                   | **6753-98-6**| A 7         | 8          | **8**    | 0                 |
| Isobutane                    | 75-28-5   | B 1         | 8          | 15       | –7                |
| Isobutane                    | 75-28-5   | B 2         | 8          | 12       | –4                |
| α-humulene                   | 6753-98-6 | B 3         | 8          | 9        | –1                |
| 1-butanol                    | 71-36-3   | B 4         | 8          | 8        | 0                 |
| Dihydromethylcyclopentapyrazine| 23747-48-0| C 1         | 8          | No ODT   |                   |
| Isopropyl alcohol            | 67-63-0   | C 2         | 8          | 15       | –7                |
| Ethyl lactate                | 97-64-3   | C 3         | 8          | 6        | +2                |
| Sabine                     | 3387-41-5 | A 1         | 9          | No ODT   |                   |
| α-terpinene                  | 99-86-5   | A 2         | 9          | No ODT   |                   |
| Myrcene                     | 123-35-3  | A 3         | 9          | 1        | +8                |
| Methyl acetate               | 79-20-9   | A 4         | 9          | No ODT   |                   |
| 4-methyldecane               | 2847-72-5 | A 5         | 9          | No ODT   |                   |
| **Methyl acetate**           | **79-20-9**| A 6         | 9          | No ODT   |                   |
Table 6 (continued)

| Compound             | CAS    | Sample code | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|----------------------|--------|-------------|------------|----------|------------------------------------------|
| β-caryophyllene      | 87-44-5| A           | 7          | 9        | 5                                        |
| Limonene             | 138-86-3| B           | 1          | 9        | 6                                        |
| Isobutyraldehyde     | 78-84-2| B           | 2          | 9        | 3                                        |
| Alloaromadendrene    | 25246-27-9| B   | 3          | 9        | No ODT                                  |
| β-caryophyllene      | 87-44-5| B           | 4          | 9        | 2                                        |
| Ethyl lactate        | 97-64-3| C           | 1          | 9        | 8                                        |
| Ethyl lactate        | 97-64-3| C           | 2          | 9        | 10                                       |
| δ-3-carene           | 13466-78-9| C   | 3          | 9        | 12                                       |
| β-caryophyllene      | 87-44-5| A           | 1          | 10       | 4                                        |
| (+)-4-Carene         | 29050-33-7| A   | 2          | 10       | 16                                       |
| α-terpinyl acetate   | 80-26-2| A           | 3          | 10       | No ODT                                  |
| Fenchyl alcohol      | 1632-73-1| A        | 4          | 10       | No ODT                                  |
| Benzaldehyde         | 100-52-7| A           | 5          | 10       | 14                                       |
| Valencene            | 4630-07-3| A       | 6          | 10       | No ODT                                  |
| 2-chloroacetophenone | 532-27-4| A           | 7          | 10       | 3                                        |
| Camphene             | 79-92-5| B           | 1          | 10       | No ODT                                  |
| Tyramine             | 51-67-2| B           | 2          | 10       | No ODT                                  |
| Isobornyl thiocyanatoacetate | 115-31-1| B   | 3          | 10       | No ODT                                  |
| Longifolene          | 475-20-7| B           | 4          | 10       | No ODT                                  |
| δ-3-carene           | 13466-78-9| C   | 1          | 10       | 14                                       |
| Propylene glycol     | 57-55-6| C           | 2          | 10       | No ODT                                  |
| α-terpinene          | 99-86-5| C           | 3          | 10       | No ODT                                  |

Sample code, see Section 1.5, corresponding to sample identification. ODT = odor detection threshold from Devos et al. [5].

Table 7

Comparing rank of top 10 most concentrated VOCs with the calculated OAV in all cocaine samples. Bolded font signifies 1 g real cocaine (sample code D4/D5). Underlined font signifies 1 g surrogate cocaine (sample code E1).

| Compound             | CAS    | Sample Code | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|----------------------|--------|-------------|------------|----------|------------------------------------------|
| Isobutanol           | 78-83-1| D           | 1          | 1        | 37                                       |
| Isobutyraldehyde     | 78-84-2| D           | 2          | 1        | 1                                        |
| Acetic acid          | 64-19-7| D           | 3          | 1        | 2                                        |
| Acetic acid          | 64-19-7| D           | 4          | 1        | 1                                        |
| Acetic acid          | 64-19-7| D           | 5          | 1        | 1                                        |
| Methyl benzoate      | 93-58-3| E           | 1          | 1        | 1                                        |
| n-Propyl acetate     | 109-60-4| D       | 1          | 2        | 8                                        |
| Isobutane            | 75-28-5| D           | 2          | 2        | 7                                        |
| n-Propyl acetate     | 109-60-4| D       | 3          | 2        | 9                                        |
| Ethylene oxide       | 75-21-8| D           | 4          | 2        | 23                                       |
| n-Propyl acetate     | 109-60-4| D       | 5          | 2        | 2                                        |
| Isobutyrophenone     | 611-70-1| E           | 1          | 2        | 12                                       |
| Acetone              | 67-64-1| D           | 1          | 3        | 20                                       |
| 4-methyldecane       | 2847-72-5| D      | 2          | 3        | 17                                       |
| Phenylethyl alcohol  | 60-12-8| D           | 3          | 3        | 1                                        |
| n-Propyl acetate     | 109-60-4| D           | 4          | 3        | 4                                        |
| Ethylacetate         | 141-78-6| D           | 5          | 3        | 10                                       |
| Ethylene oxide       | 75-21-8| E           | 1          | 3        | 8                                        |
| Butane               | 106-97-8| D           | 1          | 4        | 30                                       |
| 2-methylpentane      | 107-83-5| D           | 2          | 4        | 18                                       |
| Toluene              | 108-88-3| D           | 3          | 4        | 10                                       |
| Ethylacetate         | 141-78-6| D           | 4          | 4        | 8                                        |
| 2-butanone           | 78-93-3| D           | 5          | 4        | 12                                       |
| 2-chloroacetophenone | 532-27-4| E           | 1          | 4        | 3                                        |
| Tetradecane          | 629-59-4| D           | 1          | 5        | 38                                       |

S. Rice, J.A. Koziel / Data in Brief 5 (2015) 653–706
| Compound                  | CAS          | Sample Code | Rank conc. | Rank OAV | Change in ranking (Rank Conc. – Rank OAV) |
|---------------------------|--------------|-------------|------------|----------|------------------------------------------|
| 3,4,5-trimethyl-1-hexene  | 56728-10-0   | D 2         | 5          | 19       | –14                                      |
| 2-chloroacetophenone      | 532-27-4     | D 3         | 5          | 3        | +2                                       |
| Diacetonitrile            | 123-42-2     | D 4         | 5          | 7        | –2                                       |
| Diacetone alcohol         | 123-42-2     | D 5         | 5          | 8        | –3                                       |
| Dodecane                  | 112-40-3     | E 1         | 6          | 10       | –1                                       |
| Ethylacetate              | 141-78-6     | D 1         | 6          | 9        | –3                                       |
| Isopropyl alcohol         | 67-63-0      | D 2         | 6          | 4        | +2                                       |
| Acetone                   | 67-64-1      | D 4         | 6          | 14       | –8                                       |
| Ethyl octanoate           | 106-32-1     | E 1         | 7          | 1        | +6                                       |
| Propanoic acid            | 79-09-4      | D 1         | 8          | 1        | +6                                       |
| Ethanol                   | 64-17-5      | D 2         | 7          | 11       | –4                                       |
| 2-ethylhexanol            | 104-76-7     | D 3         | 7          | 7        | 0                                        |
| 1,2-diethylhydrazine      | 1615-80-1    | D 4         | 7          | 29       | –22                                      |
| Ethyl lactate             | 97-64-3      | D 5         | 7          | 13       | –6                                       |
| Decane                    | 124-18-5     | E 1         | 7          | 7        | 0                                        |
| Methyl benzoate           | 93-58-3      | D 1         | 8          | 5        | +3                                       |
| Propylene glycol          | 57-55-6      | D 2         | 8          | 20       | –12                                      |
| 2-butanone                | 78-93-3      | D 3         | 8          | 18       | –10                                      |
| Isopropyl alcohol         | 67-63-0      | D 4         | 8          | 16       | –8                                       |
| Hexane                    | 110-54-3     | D 5         | 8          | 21       | –13                                      |
| 1-undecanol               | 112-42-5     | E 1         | 8          | 5        | +3                                       |
| 2-chloroacetophenone      | 532-27-4     | D 1         | 9          | 2        | +7                                       |
| Acetone                   | 67-64-1      | D 2         | 9          | 10       | –1                                       |
| Ethylacetate              | 141-78-6     | D 3         | 9          | 13       | –4                                       |
| Propylene glycol          | 57-55-6      | D 4         | 9          | 30       | –21                                      |
| Methyl thioycanate        | 556-64-9     | D 5         | 9          | 5        | +4                                       |
| Cyclohexane               | 110-82-7     | E 1         | 9          | 11       | –2                                       |
| Isobutyrophenone          | 611-70-1     | D 1         | 10         | 39       | –29                                      |
| methylhydrazine           | 60-34-4      | D 2         | 10         | 21       | –11                                      |
| Isobutylaldehyde          | 78-84-2      | D 3         | 10         | 5        | +5                                       |
| 2-Hydroxyethylethydrazine | 109-84-2     | D 4         | 10         | 31       | –21                                      |
| Isopropyl alcohol         | 67-63-0      | D 5         | 10         | 20       | –10                                      |
| Acetone                   | 67-64-1      | E 1         | 10         | 10       | 0                                        |

Code, see Section 1.5, corresponding to sample identification. ODT = odor detection threshold from Devos et al., [5].
Table 8
Comparing rank of top 10 most concentrated VOCs with the calculated OAV in all heroin samples. Bolded font signifies 1 g real heroin (sample code F1/F2). Underlined font signifies 1 g surrogate marijuana (sample code G1).

| Compound                  | CAS          | Sample Code | Rank conc. | Rank OAV | Change in ranking |
|---------------------------|--------------|-------------|------------|----------|-------------------|
|                           |              |             |            |          | (Rank Conc. – Rank OAV) |
| Acetic acid               | 64-19-7      | F 1         | 1          | 1        | 0                 |
| Isobutyraldehyde          | 78-84-2      | F 2         | 1          | 1        | 0                 |
| Acetic acid               | 64-19-7      | G 1         | 1          | 1        | 0                 |
| Ethylene oxide            | 75-28-5      | F 2         | 2          | 12       | –10               |
| Isobutane                 | 78-84-2      | F 1         | 3          | 4        | –1                |
| 4-methyldecane            | 2847-72-5    | F 2         | 3          | 9        | –6                |
| Cyclohexane               | 110-82-7     | G 1         | 3          | 0        | 0                 |
| Isobutane                 | 75-28-5      | F 1         | 4          | 9        | –5                |
| 2-methylpentane           | 107-83-5     | F 2         | 4          | 0        | No ODT            |
| Methyl benzoate           | 93-58-3      | G 1         | 4          | 4        | 0                 |
| 4-methyldecane            | 2847-72-5    | F 1         | 5          | 0        | No ODT            |
| 3,4,5-trimethyl-1-hexene  | 56728-10-0   | F 2         | 5          | 0        | No ODT            |
| Ethyl cyclohexane         | 1678-91-7    | G 1         | 9          | 0        | No ODT            |
| 2-methylpentane           | 107-83-5     | F 1         | 6          | 3        | No ODT            |
| Ethylenimine              | 151-56-4     | F 2         | 6          | 0        | No ODT            |
| 1-butanol                 | 71-36-3      | G 1         | 7          | 1        | –1                |
| Butyric acid              | 107-92-6     | F 1         | 7          | 2        | +5                |
| 2,3-dimethylbutane        | 79-29-8      | F 2         | 7          | 0        | No ODT            |
| 2-chloroacetophenone      | 532-27-4     | G 1         | 7          | 3        | +4                |
| Pentanoic acid            | 109-52-4     | F 1         | 8          | 3        | +5                |
| Acetone                   | 67-64-1      | F 2         | 8          | 0        | +2                |
| Benzaldehyde              | 100-52-7     | G 1         | 8          | 6        | +2                |
| 3,4,5-trimethyl-1-hexene  | 56728-10-0   | F 1         | 9          | 0        | No ODT            |
| 3-methylhexane            | 589-34-4     | F 2         | 9          | 0        | No ODT            |
| p-cymene                  | 99-87-6      | G 1         | 9          | 2        | +7                |
| Acetone                   | 67-64-1      | F 1         | 10         | 11       | –1                |
| Acetic acid               | 64-19-7      | F 2         | 10         | 2        | +8                |
| 1,2,3,4-tetramethylbenzene| 488-23-3     | G 1         | 10         | 2        | +5                |

Code, see Section 1.5, corresponding to sample identification. ODT = odor detection threshold from Devos et al. [5].

Acknowledgments

The authors would like to acknowledge Iowa Division of Criminal Investigation, Drug Identification Section, for providing samples tested in this study.

References

[1] S. Rice, J.A. Koziel, The relationship between chemical concentration and odor activity value explains the inconsistency in making a comprehensive surrogate scent training tool representative of illicit drugs, Forensic Sci. Int. 257 (2015) 257–270 10.1016/j.forsciint.2015.08.027.
[2] S. Rice, Investigating the Aroma of Marijuana, Cocaine, and Heroin for Forensic Applications Using Simultaneous Multidimensional Gas Chromatography – Mass Spectrometry – Olfactometry, Department of Agricultural and Biosystems Engineering, 2015.
[3] CAS (Chemical Abstracts Service), The American Chemical Society, Available from: (www.cas.org) (accessed 18.08.15).
[4] G. Leonards, D. Kendall, N. Barnard, Odor threshold determinations of 53 odorant chemicals, J. Air Pollut. Control. Assoc. 19 (1969) 91–95.
[5] M. Devos, F. Patte, J. Rouault, P. Laffort, L.J. Van Gemert, Standardized Human Olfactory Thresholds, IRL Press at Oxford Press. Print, NY, New York, 1990.
[6] R. Mottram, LRI & Odour Database, Available from: (www.odour.org.uk/index.html) (accessed 08.08.14).
[7] T.E. Acree, H. Arn, Flavornet and human odor space, 2004, Available from: [http://flavornet.org/flavornet.html] (accessed 08.08.14).

[8] TGSC, The Good Scents Company Information System, Available from: [http://www.thegoodscentcompany.com/index.html] (accessed 08.09.14).

[9] D.H. Passe, J.C. Walker, Odor psychophysics in vertebrates, Neurosci. Biobehav. Rev. 9 (1985) 431–467.

[10] W. Neuhaus, Uber die Riechscharfe des Hundes fur Fettsauren, Z. Vergl. Physiol. 53 (1953) 527–552.

[11] E.H. Ashton, J.T. Eayrs, D.G. Moulton, Olfactory acuity in the dog, Nature 179 (1957) 1069–1070.

[12] D.G. Moulton, E.H. Ashton, J.T. Eayrs, Studies in olfactory acuity, 4. Relative detectability of n-aliphatic acids by the dog, Anim. Behav. 8 (1960) 117–128.

[13] D.G. Moulton, D.A. Marshall, The performance of dogs in detecting a-ionone in the vapor phase, J. Comp. Physiol. 110 (1976) 287–306.

[14] D.A. Marshall, L. Blumer, D.G. Moulton, Odor detection curves for n-pentanoic acid in dogs and humans, Chem. Senses 6 (1981) 445–453.

[15] D. Krestel, D. Passe, J.C. Smith, L. Jonsson, Behavioural determination of olfactory thresholds to amyl acetate in dogs, Neurosci. Biobehav. Rev. 8 (1984) 169–174.

[16] N. Lorenzo, T. Wan, R.J. Harper, Y.L. Hsu, M. Chow, S. Rose, K.G. Furton, Laboratory and field experiments used to identify Canis lupus var. familiaris active odor signature chemicals from drugs, explosives, and humans, Anal. Bioanal. Chem. 376 (2003) 1212–1224.

[17] M. Williams, J.M. Johnston, Training and maintaining the performance of dogs (Canis familiaris) on an increasing number of odor discriminations in a controlled setting, Appl. Anim. Behav. Sci. 78 (2002) 55–65.