Supplementary Information: Comprehensive characterization of mainstream marijuana and tobacco smoke

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S1 Cigarette samples

The tobacco cigarettes smoked were 3R4F reference cigarettes (Kentucky Tobacco Research & Development Center, USA)¹. Each 3R4F tobacco sample consists of 0.775 g of tobacco in a 57 mm long rod with a circumference of 24.8 mm¹. A 27 mm long cellulose acetate filter forms the remainder of the 84 mm cigarette length. Smoking one 3R4F reference cigarette produces 0.73 mg of nicotine and 9.4 mg of tar¹. The Kentucky reference tobacco products are designed to represent tobacco products of US consumers without any additional flavorings, with the 3R4F cigarette being more representative of the most popular tobacco cigarettes available in the US and having a stock-level of approximately 28 million². Due to this wide-acceptance by researchers in this field, using a reference cigarette allows comparison of the results not just within this study, but between data collected in different studies, including those with different tobacco products².

The marijuana cigarettes smoked were ACES pre-rolled joints with milled sativa flower (Aurora Cannabis Inc., Edmonton, Canada). Neglecting the twisted paper end, each joint was approximately 90 mm long (6 mm longer than the 3R4F cigarette), including the cardboard tipping paper that was approximately 27 mm long (similar length as the 3R4F cellulose filter). Since no standard or reference joint exists, the ACES were chosen as the best alternative since (a) they contained milled Cannabis sativa flower, a common strain of marijuana, (b) they each contained 0.5 g of marijuana, a common mass for marijuana joints and the closest in size to the 3R4F tobacco cigarettes, (c) they were pre-rolled by machine to minimize variability between samples, (d) they are produced by the second largest cannabis company in the world by market capitalization (at the time of writing), (e) they are available for purchase direct to private consumers from provincial governments in Canada (from at least six provinces representing over 88% of the population of Canada³). Based on the Aurora product labelling, smoking one ACES joint produces 88.0 mg of THC (accounting for the decarboxylation of the THC-A during combustion) and 0 mg of CBD.

From the introduction of filtered cigarettes in the 1950s, their market share grew to more than 97% by the mid 1990s in the United States⁴,⁵, United Kingdom⁵ and Japan⁶. In 2016, filtered cigarettes accounted for 99.7% of the cigarettes purchased in the United States⁴. However, marijuana is smoked differently than cigarettes, usually without a filter⁷–¹⁰, down to a smaller butt⁹,¹¹–¹³ and using longer/deeper inhalation techniques⁹,¹²,¹⁴,¹⁵. Of the thirteen provinces or territories in Canada, ten currently provide online government dispensaries, with nine dispensaries offering 244 pre-rolled products¹⁺ at the time of writing. Eight of these nine government dispensaries were contacted¹, with three dispensaries confirming that all 61 pre-rolled products offered were nonfiltered (i.e. cardboard tipping paper). Based on online photos and descriptions of the other 183 pre-rolled products offered by the five other dispensaries, only two products were filtered. Therefore, approximately 99% of the pre-rolled marijuana joints currently offered across Canada are nonfiltered (i.e. cardboard tipping paper). To represent the most common consumption methods, this study compares the smoke produced from a filtered tobacco cigarette with that from a nonfiltered marijuana joint.

S2 Smoke generation and sampling

Smoke was produced from either tobacco cigarettes or marijuana joints using a Smoking Cycle Simulator machine (SCS; Cambustion Ltd., Cambridge, UK) as shown in Fig. S1. The SCS controlled the inhalation pattern during smoking using the
Health Canada Intense (HCI) puffing parameters (55 mL puff of 2 s duration, every 30 s, for 8 puffs)\textsuperscript{16}. HCI was selected as it is a compromise between the ISO standard\textsuperscript{17} puff routine (35 mL puff of 2 s duration, every 60 s, for 8 puffs) commonly used for tobacco cigarette smoking and the more aggressive routine (70 mL puff of 2 s duration, every 30 s, for 8 puffs) developed by Moir et al.\textsuperscript{14} to represent the longer/deeper inhalation techniques used during marijuana joint smoking\textsuperscript{9–12,14,15}.

For aerosol characterization, mainstream smoke was sampled from the cigarette or joint through the heated puff head into a cylindrical lung bag (6.4 cm diameter and 35 cm length). Immediately prior to starting the puff routine, the lung bag was pre-filled using the heated breath head with 300 mL of HEPA-filtered air to act as a buffer volume during smoke generation. To limit smoke particle coagulation during the puff routine, 297 mL of HEPA-filtered dilution air was also added to the lung bag immediately prior to each 55 mL puff. The 355 mL volume (i.e. combined smoke and dilution air volume added) present in the lung bag after each puff was transferred through the heated breath head into a cylindrical sample bag (29.1 cm diameter and 100 cm length) between each puff. At the end of the puff routine, the remaining volume in the lung bag (i.e. last puff with dilution air and buffer air) was transferred to the sample bag. Prior to connecting to the SCS, the sample bag was manually pre-filled with 30 L of HEPA-filtered dilution air to provide sufficient volume for sampling with the particle characterization equipment. The lung and sample bag were both replaced between each cigarette or joint smoked, and were made of medium-duty (62.5 micron thick), polyethylene tubing (Kite Packing, Coventry, UK) with one end heat sealed. To avoid cross-contamination, the smoke generation apparatus was cleaned at the start of each day or when switching between smoking tobacco or marijuana samples.

For chemical analyses and total particulate matter (TPM) measurements, the non-vapor component of the smoke produced was sampled using quartz filters which were mounted in a stainless steel filter holder attached to the heated SCS puff head. This setup captured mainstream smoke directly from the mouth end of the cigarette or joint, therefore limiting sample losses and phase re-partitioning. During this filter loading, the stainless filter holder was cleaned between each cigarette or joint smoked and no lung and sample bag were required.

The filters (for chemical analyses and TPM measurements), cigarettes and joints were conditioned prior to sampling at a temperature of 22±1 °C and relative humidity of 60±3% for a minimum of 48 hours, in line with the ISO standard for tobacco conditioning and testing\textsuperscript{18}. Flameless ignition was achieved using a coiled electric heater with a flat surface.

**S3 Aerosol analyses**

To assess some of the effects of the steady-state sampling on the smoke characteristics, the diffusion and settling losses of the particles during the aerosol analyses were estimated. The particle losses in each aerosol instrument was considered within its standard inversion procedure (i.e. SMPS correction following TSI\textsuperscript{19} or AAC correction following Johnson et al.\textsuperscript{20}) or accounted for based on a previous study (i.e. catalytic stripper correction following Dickau et al.\textsuperscript{21}). The other aerosol measurements (i.e. particle mass, effective density and semi-volatile fraction) did not require corrections for particle losses in the DMA, CPMA or catalytic stripper as the results only depended on the location of the measurement peak in the mobility or mass domain, not its amplitude.

The particle losses in the sample bag were estimated following a similar approach as Johnson et al.\textsuperscript{22}, which is based on the aerosol theory summarized by Hinds.\textsuperscript{23} The diffusion and losses in the sample bag were found to be insignificant to the lognormal parameters (< 5.5% change) of the smoke size distributions. As expected, these corrections slightly increased the amplitudes of both the lower (i.e. diffusion losses) and upper (i.e. settling losses) extremities of the size distributions. As a result, the GSD and N for both the mobility and aerodynamic size distributions increased slightly, between 0.3-1.0% and 2.2-3.7%, respectively, for all but one smoke sample. The nonstripped marijuana smoke, with its larger particles, had slightly higher settling losses in the sample bag with the GSD and N of both the mobility and aerodynamic size distributions increasing
between 1.1-1.3% and 4.4-5.5%, respectively. Due to these loss corrections being relatively symmetric, the CMDs of both the mobility and aerodynamic size distributions remained the same (<2% change) for all of the smoke samples.

Furthermore, these changes in the size distribution are likely overestimated due to the loss estimates being conservative. The losses were estimated assuming the particle concentration remained constant in the sample bag and that the aerosol sample remained in the bag for 15 minutes before being sampled. In reality, the particle concentration in the bag decreases over time due to particle coagulation (as summarized in the Discussion section of the main text) and a portion of particles were sampled immediately after the puff routine finished. To further limit particle losses, the SMPS voltage was scanned upwards to measure the smallest particles first (i.e. where diffusion losses increase), and the AAC speed was stepped upwards to measure the largest particles first (i.e. where settling losses increase). These negligible losses of particles also agree with the insignificant diffusion and settling losses estimated by Johnson et al.\textsuperscript{22} for nonstripped tobacco smoke in a 10 L sample bag. Since these loss estimates are conservative, are based on simplifying assumptions and are negligible relative to the other uncertainties of the measurements (as summarized in the Statistical Analysis section of the main text), these loss corrections were not applied to the results presented in this study.

**S3.1 Measurement of aerosol size distributions**

The setup used to measure the particle size distributions is shown in Fig. S2. An aerosol sample flow was drawn from the sample bag at 0.6 L min\(^{-1}\). This sample flow was first passed through a catalytic stripper (Catalytic Instruments GmbH & Co.KG, Rosenheim, Germany: Model CS015) operated with an internal gas temperature of 350\(^\circ\)C (i.e. hot condition) or 21\(^\circ\)C (i.e. cold condition). Under the hot catalytic stripper condition, the semi-volatile component of the aerosol was removed\textsuperscript{24}, whereas in the cold catalytic stripper, the semi-volatile component remained. The difference in particle losses within the catalytic stripper between the hot and cold operating conditions were corrected for following Dickau et al.\textsuperscript{21}.

The aerosol sample flow was then split, with 0.3 L min\(^{-1}\) drawn to a condensation particle counter (CPC), labelled as CPC 1 in Fig. S2. The CPC quantifies the particle number concentration of the aerosol by condensing butanol on the particles to generate droplets (several microns in diameter) large enough to be detected optically\textsuperscript{25}. Due to this operating principle with the consistent working fluid, the CPC measurements are insensitive to the refractive index of the particles. The remaining 0.3 L min\(^{-1}\) sample flow was used to measure either the aerodynamic or mobility particle size distribution.

To measure the aerodynamic size distributions of the aerosol samples, an aerodynamic aerosol classifier (AAC; Cambustion Ltd.) and a CPC were used\textsuperscript{20}. The AAC uses a centrifugal force to move particles that are in-turn resisted by their drag force in the carrier gas. Only particles with a narrow range of aerodynamic (-equivalent) diameters follow the correct trajectory and pass through the AAC\textsuperscript{26}. This aerodynamic diameter setpoint can be set anywhere between 25 nm and 6.8 \(\mu\)m by varying the classifier speed and gas flows of the AAC\textsuperscript{27}. At the flow rates used in this study, 0.3 and 3 L min\(^{-1}\) for the sample and sheath flow\textsuperscript{1}, respectively, the classification range of the AAC was approximately 30 nm to 2.86 \(\mu\)m. By measuring the classified particle concentrations using a CPC (labelled CPC 2 in Fig. S2) as the AAC setpoint is stepped, the aerodynamic size distribution of an aerosol can be quantified\textsuperscript{20}. These aerodynamic size distribution measurements were repeated three times, each from a new sample bag, and averaged to generate the size distribution parameters reported in Fig. 1a and in-text.

\textsuperscript{1}These classifier flow rates correspond to a classification resolution of 10.
Both CPCs shown in Fig. S2 and used in the other experimental setups for the aerosol portion of this study were the same model (TSI Inc., Shoreview, MN, USA: Model 3776) and detect particles with diameters from 2.5 nm to 3 μm. Since the particle number concentrations in the sample bag decreased over time and the AAC scans were approximately 15 mins long, the particle number concentrations upstream of the AAC (measured by CPC 1) were used to normalize those downstream of the AAC (measured by CPC 2). This correction method was also utilized by Johnson et al. for effective density measurements of aged tobacco smoke particles.

To measure the mobility size distributions of the aerosol samples, a Scanning Mobility Particle Sizer was used (SMPS; TSI Inc.: 3077 Bipolar charge conditioner, 3080 Electrostatic Classifier, 3081 Differential Mobility Analyzer [DMA], 3776 Condensation Particle Counter [CPC]). A bipolar charge conditioner was placed upstream of the DMA to charge the aerosol to a known equilibrium distribution of electrical charges. The DMA uses an electrostatic force to move the charged particles that are in-turn resisted by their drag force in the carrier gas. Only particles with a narrow range of mobility (equivalent) diameters follow the correct trajectory and pass through the DMA. This mobility diameter setpoint can be set anywhere between 10 nm and 1 μm by varying the classifier voltage and gas flows of the DMA. At the flow rates used in this study, 0.3 and 3 L min⁻¹ for the sample and sheath flow, respectively, the classification range of the DMA operating within an SMPS over a 120 second scan was approximately 15 to 685 nm.

By measuring the classified particle concentrations using a CPC (labelled CPC 2 in Fig. S2) as the DMA setpoint is scanned, the mobility size distribution of an aerosol can be quantified. This measured distribution was corrected for multiply-charged particles following He & Dhaniyala. The five consecutive mobility size distribution measurements (i.e. consecutive three minute scans started after the puff routine finished) were repeated three times, each from a new sample bag, and averaged to generate the size distribution parameters reported in Fig. 1b and in-text. The mobility scan shown in Fig. 1b is an average of all fifteen SMPS scans, accounting for the change in the smoke particle concentration over time by scaling the entire distribution by its total particle concentration relative to that from the first scan.

Both the aerodynamic and mobility particle size distributions were characterized by a log-normal distribution using a least-squares regression to determine the fitted count median diameter (CMD), geometric standard deviation (GSD), and total number concentration. These measurements focused on the measured CMD and GSD of the smoke particles, as the total particle number concentrations quantified by these methods were limited due to the transient nature of the smoke particles as discussed in the next section.

### S3.2 Measurement of total number concentration

The particle number concentration of each aerosol sample was directly measured as a function of time using CPC 1 as labelled in Fig. S2. The particle number concentration was also indirectly measured by integrating the area under the aerodynamic or mobility size distributions.

The measured particle number concentration decreased over time as shown in Fig. S3 and Fig. S4. These concentrations are corrected for the sample dilution factor of 75 which accounts for the 30 L of dilution air in the sample bag, and 297 mL of dilution air per puff and 300 mL of buffer dilution air added into the lung bag.

Fig. S4 shows the mobility size distributions of the nonstripped tobacco smoke particles measured by the SMPS as a function of time. This measurement demonstrates that the mobility CMD remained relatively constant (within 1.4% of the average CMD of nonstripped tobacco smoke) between the 5 consecutive 3 minute scans (i.e. 15 minute total measurement time). The change in the mobility CMD over the 5 consecutive mobility scans from either smoke source and condition (nonstripped vs stripped) varied by less than 5.4% over a similar period.

All three measurement methods of particle concentration varied due to the transient nature and high concentration of the smoke particles. The reported CPC 1 measurements include a coincidence correction as the measured particle concentrations were greater than 3 × 10⁵ particles cm⁻³, a threshold above which the CPC has reduced measurement accuracy. Furthermore, CPC 1 was measuring at the maximum of its range (1 × 10⁶ particles cm⁻³) for the first 0 to 15 seconds of sampling depending on the smoke source and its conditioning (nonstripped or stripped). It should be noted that these conditions did not occur in CPC 2 as the particle concentrations were below the CPC coincidence correction threshold after classification by the AAC, DMA, or CPMA. The number concentrations determined from the mobility measurements are sensitive to the SMPS multiple-charge correction. Furthermore, the common practice for characterizing steady-state aerosols (as alluded to in Annex G of BS ISO 15900) is to use a SMPS to measure the mobility size distribution and in parallel use a CPC to measure the total particle number concentration since charge corrections are not required for a CPC. While the aerodynamic measurements do not require a multiple charge correction, its long scan time (~15 minutes) of a transient aerosol likely had the greatest effect on the area under the measured aerodynamic size distribution. This inference is supported by the stability of the mobility CMD between consecutive SMPS measurements. However, despite these additional sources of concentration measurement errors, the particle

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8 Assuming the particles are singly charged.
**Figure S3.** Change in particle number concentration of nonstripped tobacco and marijuana smoke over time.

**Figure S4.** Change in mobility size distribution of nonstripped tobacco smoke over time. Total number concentration reduces over time and mean diameter remains relatively constant.
Figure S5. Experimental setups for measurement of size-selected effective density and size-selected semi-volatile volume fraction of smoke particles using (a) nonstripped and (b) stripped particles.

centre of mass ratio between marijuana and tobacco smoke from all three measurement methods agreed within 20% for both nonstripped and stripped aged smoke samples as shown in Fig. 1c and in-text.

S3.3 Measurement of effective density

Effective density of nonstripped smoke particles as a function of particle mobility diameter was measured using the setup shown in Fig. S5a. Similar to the experimental setups for aerosol size distribution measurements, a sample flow rate of 0.6 L min$^{-1}$ was used. However, in this case, the smoke particles were first classified by mobility using DMA 1 at a constant diameter setpoint prior to a second aerosol classifier. Similar to the previous setups, the sample flow was split, with 0.3 L min$^{-1}$ drawn by CPC 1 to measure the total number concentration of the classified particles (i.e. downstream of DMA 1), which were monodispersed in electrical mobility. The remaining 0.3 L min$^{-1}$ classified sample flow was passed through a centrifugal particle mass analyzer (CPMA) to classify the particles by their mass-to-charge ratio using opposing centrifugal and electrostatic forces generating by charged, rotating concentric cylinders$^{34}$. This mass-to-charge setpoint$^6$ can be set anywhere between 0.2 ag and 1050 fg by varying the classifier speed and voltage of the CPMA$^{35}$. At the sample flow of 0.3 L min$^{-1}$ and the classification resolution of 20 used in this study, the classification range of the CPMA was approximately 3.8 ag to 296 fg. The CPMA was operated at twice the classification resolution of the AAC or DMA (i.e. 20 vs 10) to further distinguish the charge states of the particles classified by the upstream DMA.

By measuring the classified particle concentrations using a CPC (labelled CPC 2 in Fig. S5a) as the CPMA setpoint is stepped, the mass-to-charge distribution of an aerosol can be quantified$^{36,37}$. Since the charge states of the particles are known from the upstream neutralizer and DMA, the particle mass classified by the CPMA at the given DMA setpoint can be determined. Using the measured particle mass and mobility diameter, the effective density of the particles can be calculated following Eqn. 1 of main-text.

The effective densities of stripped particles were measured using the setup shown in Fig. S5b. The 0.6 L min$^{-1}$ sample classified by DMA 1, which was monodispersed in particle mobility, was passed through a catalytic stripper at 350°C. The
effective density of the particles was measured by using the two downstream classifiers, DMA 2 and the CPMA, in parallel to measure the mobility diameter and mass of the stripped particles, respectively. Each downstream classifier was operated in tandem with a CPC operating at at 0.3 L min$^{-1}$. Due to this tandem classifier arrangement, DMA 2 was not operated in scanning mode like an SMPS to avoid introducing additional errors into its mobility measurements. These errors are caused by the upstream DMA (i.e. DMA 1) producing a narrow mobility distribution, which invalidates the SMPS inversion assumption that the aerosol distribution is constant over the width of the downstream DMA (i.e. DMA 2) transfer function$^{38}$. To avoid this issue, the downstream DMA was stepped, rather than scanned, and the tandem DMA inversion developed by Stolzenburg & McMurry$^{39}$ was applied. This tandem DMA inversion was also previously used to study the hygroscopic properties of tobacco smoke particles$^{40}$.

For both the nonstripped and stripped smoke samples, this process was repeated at various particle sizes (i.e. different DMA setpoint) to identify the relationship between particle mobility diameter and effective density as shown in Fig. 1d and in-text.

### S3.4 Measurement of total particulate matter
The total particulate matter (TPM) produced by smoking a tobacco cigarette or marijuana joint was measured by collecting fresh smoke (i.e. without dilution or aging) on a quartz filter directly downstream of the cigarette or joint. The quartz filters (47 mm Type A/E Glass Fiber Filter from Pall Life Sciences [P/N 61631]) were weighed before and after loading using an ultra-microbalance (UMX2; Mettler Toledo, Columbus, Ohio, USA). To avoid the TPM filters becoming overloaded and causing the puff routine to deviate significantly, only six of the eight puffs of the HCI smoking routine were used during the TPM filter loading for both the tobacco and marijuana samples. A TPM sample was deemed acceptable if the total puff volume was within 10% of the 330 cm$^3$ target. The total puff volumes deviated by -0.6% to -3.2% for the TPM filters loaded with tobacco smoke, and by 0.2% to -8.7% for those loaded with marijuana smoke. These deviations are on the same order of magnitude as the uncertainty of other studies, such as the 5% to 7% confidence interval calculated from the data of Moir et al.$^{14}$, which had a larger TPM sample size of 30 repeats.

Immediately after loading the filters were placed on the ultra-microbalance, however each filter’s mass would continue to decrease for tens of minutes. This decrease was small relative to the total TPM (less than 3.6%) and is likely due to the volatility of the TPM. This observation at room temperature supports the conclusion that the particles from either smoke source have a highly volatile component. The TPM filters were also conditioned before and after loading, however the change in total mass due to conditioning after loading was insignificant (less than 0.6%). Over the 6 HCI puffs, the marijuana joint produced 27 ($\pm 4$) mg of TPM, while the smoking the tobacco cigarette produced 7.8 ($\pm 0.9$) mg of TPM. The reported TPM measurement limits represent the 95% confidence of the measurement repeatability assuming a t-distribution. These results agree with the results of Ingebrethsen et al.$^{41}$, which found smoking the same 3R4F tobacco cigarette following the same HCI puff routine produced 1.0$\pm 0.3$ mg and 1.9$\pm 0.3$ mg of TPM for puff 2 and puff 5, respectively, thus agreeing with the 1.3$\pm 0.3$ mg average TPM per tobacco cigarette puff currently measured. This per puff average is only a high-level comparison as it neglects that the TPM produced changes as a function of rod length or with each puff over a smoking routine.

Based on the TPM measurements and associated confidence intervals determined in the current study, smoking a marijuana joint produces roughly 3.4 ($\pm 0.6$) times more TPM than a tobacco cigarette following the same six puff routine. This result qualitatively agrees with our observation that more than six HCI puffs from the marijuana joint would overload the TPM filter causing significant puff deviations, while no such overloading and puff deviations were observed for TPM samples loaded with up to eight HCI puffs from the tobacco cigarette. However, this 3.4 ratio is contrary to the results of Moir et al.$^{14}$, which found tobacco cigarettes and marijuana joints produce approximately the same amount of TPM per puff following either the ISO (35 ml puff over 2 seconds every 60 seconds) or extreme (70 ml puff over 2 seconds every 30 seconds) smoking routines. This difference between the studies could be due the different puffs routines used, and that the tobacco cigarettes studied by Moir et al.$^{14}$ were nonfiltered as filtered cigarettes are known to reduce the TPM produced from smoking tobacco$^5$. The inference is supported by another study$^{42}$ which found on average that mainstream smoke from a marijuana joint yields on average 2.2 times greater TPM than mainstream smoke from a filter-tipped tobacco cigarette.

### S3.5 Measurement of semi-volatile mass and volume fractions
The semi-volatile mass and volume fractions at a given aerosol particle size were measured using the setup shown in Fig. S5a and S5b. The semi-volatile mass fraction at a given particle size was measured by comparing the masses of nonstripped and stripped particles measured by the CPMA at a given DMA setpoint, in this case 470 nm mobility diameter. Specifically, the count median mass (CMM) measured by the CPMA in Fig. S5a is compared with the CMM measured by the CPMA in Fig. S5b. Each CMM was determined by fitting a log-normal distribution to each charge peak of the CPMA scan using a least-squares regression.

The semi-volatile volume fraction at a given particle size was measured by comparing the mobility-equivalent volume of nonstripped and stripped particles measured by DMA 2 at a given DMA 1 setpoint as shown in Fig. S5b. Note that DMA 2 was operated in stepping mode for the reasons described in Section S3.3. Specifically, the TDMA inversion median diameter of the...
stripped particles measured by DMA 2 is compared with the nonstripped particle size selected by DMA 1 (i.e. 470 nm mobility diameter setpoint).

The semi-volatile fractions for the polydispersed size distributions were calculated using the mass and volume concentrations of the aerosols, rather than the individual particle mass and volume. The volume and mass concentrations were estimated using the Hatch-Choate equations and the lognormal distributions fitted to the measured mobility size distributions (as described in Sections S3.1). The fitted lognormal distribution was used to account for particles smaller or larger than the SMPS measurement range (14.6 to 685.4 nm). It is clearly shown in the mobility size distributions of Fig. 1b that particles larger than the SMPS measurement range are present. The mass concentration estimate also utilized the effective density of the particles as described in Section S3.3.

S4 Chemical analyses

Volatile compounds from particulates captured in pre-fired quartz filters were sampled by headspace solid-phase microextraction (HS-SPME) followed by comprehensive two-dimensional gas chromatography with a time-of-flight mass spectrometric detector (GC×GC-TOFMS). The pre-fired quartz filters (47 mm PallFlex Tissuquartz™ 2500 QAT-UP filters from Pall Life Sciences [P/N 7202]) utilized for the chemical samples were different than the TPM filters and appeared to generate a lower pressure drop during loading. As a result, the chemical sample filters did not cause the puffs to deviate late in the smoking routine, and thus could be consistently loaded using all eight puffs for both the tobacco and marijuana samples.

S4.1 HS-SPME-GCxGC-TOFMS

The GC×GC-TOFMS system consisted of an Agilent 7890 (Agilent Technologies, Palo Alto, CA, USA) gas chromatograph and a Pegasus 4D TOFMS (LECO, St. Joseph, MI, USA) with quad jet liquid nitrogen-cooled thermal modulator. The first dimension (1D) column was a low-polarity 5% phenyl / 95% polydimethylsiloxane-type phase (Rtx-5MS; 60 m × 0.25 mm i.d.; 0.25 μm film thickness) connected by means of a SilTite μ-Union (Trajan Scientific and Medical, Victoria, Australia) to a second dimension (2D) mid-polarity trifluoropropylmethyl polysiloxane-type phase (Rxi-200; 1.6 m × 0.25 mm i.d.; 0.25 μm film thickness). Both columns were from Restek Corporation (Restek Corp., Bellefonte, PA, USA). The 2D column was installed in a separate oven located inside the main GC oven. The system was equipped with a Gerstel MultiPurpose Sampler (MPS 2XL) with SPME option for procedural automation. The carrier gas was helium at a corrected constant flow rate of 2 mL/min and the injector operated in splitless mode. The main oven temperature program was 50°C (5 min hold), a ramp of 5°C min⁻¹ to 300°C (1 min hold). The secondary oven was programmed with a constant +10°C offset relative to the primary oven. The modulation period was 2.0 s (0.3 s hot pulse and 0.7 s cold pulse time) with a +15°C offset relative to the secondary oven. Mass spectra were acquired in the range m/z 40–500 at 200 spectra s⁻¹. The ion source temperature was set at 200°C and the transfer line temperature was set at 250°C. The detector voltage was run at an offset of -200 V relative to the tuning potential and the ionization electron energy (EI source) was set at 70 eV. Samples were acquired using LECO ChromaTOF software version 4.72.0.0.

After smoking, filter pads were immediately placed in separate 20 mL headspace vials and sealed with magnetic crimp-top caps. Samples were stored in a refrigerator (≈4°C) prior to analysis. The filter pads used for this chemical sampling were pre-fired in a muffle furnace at 750°C for 4 hours. Cigarettes/joints, and filter pads were conditioned for at least 48 h at 60±3% relative air humidity and 22±1°C prior to use. Four different SPME fibre coatings were examined. The fibre coatings comprised a tri-mode (50/30 μm DVB/CAR/PDMS; divinylbenzene/carboxen on polydimethylsiloxane) fibre, a mixed-mode (65 μm PDMS/DVB; polydimethylsiloxane/divinylbenzene) fibre, a PDMS (100 μm polydimethylsiloxane) fibre, and a PA (85 μm polyacrylate) fibre, all purchased from Millipore Sigma (USA). All fibres were used to perform extractions from the headspace over the filter pads using the following conditions: an incubation time of 3 min at 70°C and an extraction time of 15 min at 70°C. The inlet temperature was maintained at 250°C during fibre desorption (2 min). Fibres were initially conditioned according to the manufacturer’s guidelines.

Data were processed using LECO ChromaTOF software version 4.71.0.0 with the following parameters. The expected peak width settings in the 1D and 2D were 12 s and 0.1 s, respectively. Peaks were detected from the raw chromatogram using a minimum signal-to-noise (S/N) ratio value of 100 with a minimum sub-peak S/N of 6. The minimum match required to combine peaks was 750. Identities of peaks were tentatively assigned on the basis of linear temperature-programmed retention indices (LTPRIs) for CS-C30 (LTPRI window ±10) and mass spectral similarity match (>750) against library spectra. Mass-spectral library searches were performed against the NIST/EPA/NIH Mass Spectral Library (NIST 17) and Wiley Registry of Mass Spectral Data (9th edition). Interactive LTPRI filters (±10) were performed by using the NIST/EPA/NIH Mass Spectral Library (NIST 17 version 2.3) as well as internet-based RI collections (i.e. PubChem) databases. Unless otherwise stated, all experiments were conducted with the aforementioned parameters. Detailed HS-SPME-GCxGC-TOFMS acquisition and data processing methods are provided at the end of the SI (SPME-GCxGC-TOFMS methods).
S4.2 SPME fibre selection

Uptake of analytes in SPME is highly dependent on the chemistry of the fibre used to perform the extraction and in this study, four different SPME fibres were investigated for their utility in profiling volatiles: polydimethylsiloxane (PDMS), polyacrylate (PA), Divinylbenzene(DVB)/PDMS, and DVB/Carboxen(CAR)/PDMS. A comprehensive profile of the compounds in the smoke is desired, while ensuring good responses for compounds that are expected to be of interest, namely the terpenes and cannabinoids. During initial development of the GC×GC method, the PDMS fibre was abandoned as it gave poor recoveries for most compounds in tobacco and marijuana smoke. Typical chromatograms for both tobacco and marijuana smoke with the various fibre chemistries tested are included in Fig. S6.

Raw chromatograms consisted of several thousand peaks for each sample with the processing method employed. In curating the peak tables, unwanted peaks such as column bleed and extra hits from tailing peaks were removed. When we considered the total number of detected compounds, the PA fibre yielded 4329 and 1936 peaks for the particulate phase fraction of mainstream tobacco smoke and mainstream marijuana smoke, respectively. Similarly, using DVB/PDMS fibre 3680 peaks in the particulate phase fraction of mainstream tobacco smoke and 1845 peaks in the particulate phase fraction of mainstream marijuana smoke were detected. When the DVB/CAR/PDMS fibre was used, the total number of compounds detected increased to 4350 and 2575 for the particulate phase fraction of mainstream smoke from tobacco and marijuana, respectively. Although these values revealed the relative differences and complexity of the tobacco smoke and marijuana smoke, the DVB/CAR/PDMS fibre shows better extraction efficiency towards a larger number of analytes with diverse chemical functionality for both sample matrices. Hence this fibre type was selected for all the subsequent analyses.
Figure S6. HS-SPME-GC×GC-TOFMS performed using three different fibres
| Chemical Class    | Tobacco | Marijuana | Common |
|------------------|---------|-----------|--------|
|                  | No. of Peaks | Total Peak Area (%) | No. of Peaks | Total Peak Area (%) | No. of Peaks | Tobacco Total Peak Area (%) | Marijuana Total Peak Area (%) |
|                  |          |              |          |                  |          |                           |                              |
| **Heterocycle**  |          |              |          |                  |          |                           |                              |
| Furan            | 19       | 1.4         | 13       | 2.6              | 8        | 1.0                        | 2.5                           |
| Pyran            | 9        | 0.6         | ND       | ND               | ND       | NF                         | NF                            |
| Pyrazine         | 16       | 0.8         | 12       | 2.1              | 9        | 0.7                        | 1.8                           |
| Pyrazole         | 1        | 0.1         | ND       | ND               | ND       | NF                         | NF                            |
| Pyridine         | 46       | 7.1         | 18       | 2.8              | 12       | 1.4                        | 2.5                           |
| Pyrimidine       | 1        | trace       | 1        | trace            | NF       | NF                         | NF                            |
| Pyrrole          | 17       | 1.1         | 17       | 2.8              | 9        | 0.5                        | 2.2                           |
| **Total**        | 109      | 12          | 61       | 10               | 38       | 3.6                        | 9.0                           |
| **Hydrocarbon**  |          |              |          |                  |          |                           |                              |
| Alicyclic        | 15       | 0.6         | 24       | 1.1              | NF       | NF                         | NF                            |
| Alkane           | 19       | 2.8         | 24       | 1.7              | 17       | 2.8                        | 1.6                           |
| Alkene           | 38       | 4.0         | 33       | 1.6              | 16       | 1.3                        | 1.0                           |
| Alkyne           | 5        | 0.2         | 1        | trace            | NF       | NF                         | NF                            |
| Diterpene        | 1        | 1.9         | 3        | 0.4              | 1        | 1.9                        | 0.4                           |
| Monocyclic Aromatic | 71       | 3.1         | 53       | 4.9              | 28       | 1.3                        | 3.3                           |
| Monoterpene      | 7        | 0.6         | 24       | 5.6              | 6        | 0.6                        | 3.0                           |
| Polycyclic Aromatic | 82       | 4.9         | 34       | 2.1              | 26       | 2.9                        | 2.0                           |
| Sesquiterpene    | 21       | 1.5         | 50       | 11               | 12       | 1.2                        | 5.1                           |
| Triterpene       | 1        | trace       | ND       | ND               | NF       | NF                         | NF                            |
| **Total**        | 260      | 18          | 246      | 28               | 106      | 12                         | 16                            |
| **Nitrogenated** |          |              |          |                  |          |                           |                              |
| Amide            | 3        | 0.3         | 1        | trace            | NF       | NF                         | NF                            |
| Amine            | 6        | 0.3         | 1        | trace            | NF       | NF                         | NF                            |
| Amino Acid       | 2        | trace       | 2        | 0.1              | 1        | trace                      | trace                         |
| Aza-arene        | 30       | 2.7         | 9        | 2.7              | 8        | 2.2                        | 2.7                           |
| Imide            | 2        | 1.9         | 2        | 0.7              | 1        | trace                      | trace                         |
| Lactam           | 1        | trace       | ND       | ND               | NF       | NF                         | NF                            |
| Nitrile          | 21       | 1.4         | 26       | 4.8              | 10       | 1.0                        | 3.6                           |
| Oxazole          | 2        | trace       | 1        | trace            | 1        | trace                      | trace                         |
| Thiazole         | 1        | trace       | ND       | ND               | NF       | NF                         | NF                            |
| **Total**        | 68       | 4.8         | 42       | 8.4              | 21       | 3.3                        | 6.4                           |
| **Oxygenated**   |          |              |          |                  |          |                           |                              |
| Alcohol          | 55       | 20          | 75       | 16               | 20       | 6.2                        | 6.2                           |
| Aldehyde         | 16       | 0.2         | 3        | trace            | 2        | trace                      | trace                         |
| Anhydride        | 1        | trace       | ND       | ND               | NF       | NF                         | NF                            |
| Cannabinoid      | ND       | ND          | 8        | 7.1              | NF       | NF                         | NF                            |
| Carboxylic Acid  | 2        | 3.2         | 2        | 2.0              | 1        | 3.1                        | 2.0                           |
| Epoxide          | 4        | 0.2         | 7        | 0.7              | NF       | NF                         | NF                            |
| Ester            | 12       | 7.0         | 27       | 1.5              | 4        | 6.2                        | 0.6                           |
| Ether            | 15       | 0.8         | 8        | 0.4              | 7        | 0.6                        | 0.4                           |
| Ketone           | 119      | 10          | 49       | 5.1              | 29       | 3.4                        | 4.3                           |
| Lactone          | 2        | 0.7         | 1        | trace            | NF       | NF                         | NF                            |
| Peroxide         | 1        | 0.1         | ND       | ND               | NF       | NF                         | NF                            |
| Quinone          | 2        | 0.3         | ND       | ND               | NF       | NF                         | NF                            |
| **Total**        | 229      | 43          | 180      | 34               | 63       | 20                         | 13                            |
| **Miscellaneous**|          |              |          |                  |          |                           |                              |
| Acetamide        | ND       | ND          | 1        | trace            | NF       | NF                         | NF                            |
| Amphetamine      | ND       | ND          | 1        | 0.1              | NF       | NF                         | NF                            |
| Carbamate        | ND       | ND          | 1        | trace            | NF       | NF                         | NF                            |
| Phosphonate      | 1        | trace       | ND       | ND               | NF       | NF                         | NF                            |
| Thiocyanate      | ND       | ND          | 1        | trace            | NF       | NF                         | NF                            |
| Trisulfide       | 1        | trace       | 1        | trace            | 1        | trace                      | trace                         |
| **Total**        | 2        | trace       | 5        | trace            | 1        | trace                      | trace                         |
| **Matrix Total** | 668      | 100         | 534      | 100              | 229      | 39                         | 45                            |
| Compound                        | Unit | RDL   | TC 1  | TC 2  | MJ 1  | MJ 2  | GC × GC TOF Only | S/N (TC) | GC × GC TOF S/N (MJ) |
|--------------------------------|------|-------|-------|-------|-------|-------|------------------|----------|-------------------|
| delta-9-Tetrahydrocannabinol   | mg   | 0.05  | <RDL  | <RDL  | 20.0  | 18.6  | -                | ND       | 9,600             |
| delta-8-Tetrahydrocannabinol   | mg   | 0.05  | <RDL  | <RDL  | <RDL  | <RDL  | X                | ND       | 2,500             |
| Cannabidiol                    | mg   | 0.05  | <RDL  | <RDL  | <RDL  | <RDL  | X                | ND       | 4,600             |
| Cannabionol                    | mg   | 0.05  | <RDL  | <RDL  | <RDL  | <RDL  | X                | ND       | 3,000             |
| Cannabigerol                   | mg   | 0.05  | <RDL  | <RDL  | <RDL  | <RDL  | X                | ND       | 500               |
| Cannabichromene                | mg   | 0.05  | <RDL  | <RDL  | <RDL  | <RDL  | X                | ND       | 22,000            |
| Nicotine*                      | µg   | 0.04  | 1040  | 1130  | <RDL  | <RDL  | -                | 24,000   | ND                |
| Acenaphthene                   | µg   | 0.5   | <RDL  | <RDL  | <RDL  | X      | 2,500            | 690      |
| Acenaphthylene                 | µg   | 0.5   | <RDL  | <RDL  | <RDL  | <RDL  | X                | 4,500    | 1,900             |
| Anthracene                     | µg   | 0.5   | <RDL  | <RDL  | <RDL  | <RDL  | X                | 670      | 870               |
| Fluorene                       | µg   | 0.5   | <RDL  | <RDL  | 0.6   | <RDL  | -                | 8,200    | 2,000             |
| Naphthalene, 1-methyl-         | µg   | 0.5   | <RDL  | <RDL  | 1.3   | 1.0   | -                | 19,000   | 7,600             |
| Naphthalene, 2-methyl-         | µg   | 0.5   | <RDL  | <RDL  | 1.8   | 1.3   | -                | 16,000   | 10,000            |
| Naphthalene                    | µg   | 0.5   | <RDL  | <RDL  | 2.3   | 1.7   | -                | 36,000   | 29,000            |
| Phenanthrene*                  | µg   | 0.5   | <RDL  | <RDL  | <RDL  | X      | 2,600            | ND       |
| Pyrene*                        | µg   | 0.5   | <RDL  | <RDL  | <RDL  | <RDL  | X                | ND       | 300               |
| Ethylbenzene                   | mg/kg| 5.0   | <RDL  | <RDL  | 10.8  | <RDL  | -                | 660      | 8,700             |
| Styrene                        | mg/kg| 5.0   | <RDL  | <RDL  | 53.9  | 13.5  | -                | 1,200    | 15,000            |
| Toluene                        | mg/kg| 5.0   | <RDL  | <RDL  | 6.4   | <RDL  | -                | ND       | ND                |
| m-Xylene                       | mg/kg| 5.0   | <RDL  | <RDL  | a     | <RDL  | X                | 1,700    | 1,300             |
| o-Xylene                       | mg/kg| 5.0   | <RDL  | <RDL  | a     | <RDL  | X                | 300      | 200               |
| p-Xylene                       | mg/kg| 5.0   | <RDL  | <RDL  | a     | <RDL  | X                | 1,000    | 4,100             |
| Formaldehyde                   | µg   | 2.5   | 14.1  | 14.5  | 17.3  | 14.8  | -                | ND       | ND                |
| Acetaldehyde (cis)             | µg   | 2.5   | 12.3  | 12.6  | 22.7  | 21.1  | -                | ND       | ND                |
| Acetaldehyde (trans)           | µg   | 2.5   | 12.0  | 12.2  | 22.1  | 20.4  | -                | ND       | ND                |

RDL is the reported detection limit of the analytical method (one-dimensional GC-MS or LC-UV) used by the contract laboratory performing quantitative analysis. Quantified compounds in two replicate samples employ the same units stated with RDL values. ND = not detected by GC × GC-TOFMS.

*Detected in tobacco only
† Detected in marijuana only
‡Reported as "xylenes" at 25.5 mg/kg by external laboratory; individual quantification was not provided
§Formaldehyde is a Group 1 carcinogen detected by external laboratory only.

Acetaldehyde is a Group 2B carcinogen (Group 1 carcinogen when associated with the consumption of alcoholic beverages) detected by external laboratory only.
Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke. G1 = Group 1 carcinogen, G2A = Group 2A carcinogen, G2B = Group 2B carcinogen, G3 = Group 3 carcinogen, M = Mutagen, T = Teratogen, X = Toxic by other mechanisms, ND = No risk data available or risks mitigated by proper protective equipment.

| Tentative Identification | CAS     | Peak Area | Health Effects | Class   | Subclass | Exp. RI† | Lib. RI‡ | Reverse†† | Similarity‡‡ |
|--------------------------|---------|-----------|----------------|---------|----------|----------|----------|-----------|--------------|
| Acetic acid              | 64-19-7 | 19571743  | -              | Oxy     | carboxylic acid | 224 | 0.37 | 60 | 650 | 649 | 983 | 981 |
| 2-Propanone, 1-hydroxy-   | 116-09-6| 4363457   | M              | Oxy     | ketone    | 278 | 0.86 | 43 | 683 | 688 | 959 | 948 |
| 2,3-Pentanedione         | 600-14-6| 127492    | -              | Oxy     | ketone    | 306 | 0.78 | 57 | 700 | 698 | 963 | 815 |
| 2-Butanone, 3-hydroxy-   | 513-86-0| 349470    | -              | Oxy     | ketone    | 326 | 0.965 | 45 | 713 | 713 | 928 | 846 |
| Butanenitrile, 3-methyl- | 625-28-5| 196831    | X              | Nit     | nitrile   | 354 | 1.14 | 43 | 730 | 730 | 869 | 818 |
| Pyridine                 | 110-86-1| 2058995   | G2B            | Het     | pyridine  | 376 | 0.68 | 79 | 743 | 746 | 936 | 937 |
| (Dimethylamino)-acetonitrile | 926-64-7| 130480    | X              | Nit     | nitrile   | 380 | 1.04 | 83 | 746 | NA  | 936 | 791 |
| 1H-pyrrole               | 109-97-7| 249200    | M              | Het     | pyrrole   | 388 | 0.58 | 67 | 750 | 755 | 968 | 833 |
| Cyclopentanone           | 120-92-3| 704948    | -              | Oxy     | ketone    | 454 | 1.05 | 55 | 791 | 791 | 980 | 951 |
| Pyridine, 2-methyl-      | 109-06-8| 1027226   | M              | Het     | pyridine  | 504 | 0.61 | 93 | 816 | 816 | 953 | 937 |
| 2-Methylpyrazine         | 109-08-0| 1098300   | M              | Het     | pyrazine  | 522 | 0.66 | 94 | 825 | 831 | 955 | 942 |
| 2-Cyclopenten-1-one      | 930-30-3| 1210377   | -              | Oxy     | ketone    | 540 | 1.24 | 82 | 834 | 834 | 951 | 934 |
| Cyclopentanone, 2-methyl-| 1120-72-5| 376556    | -              | Oxy     | ketone    | 556 | 0.96 | 42 | 841 | 843 | 944 | 922 |
| Pentanenitrile, 4-methyl-| 542-54-1| 502268    | -              | Nit     | nitrile   | 558 | 1.28 | 55 | 842 | 843 | 953 | 904 |
| Cyclopentanone, 3-methyl-| 1757-42-2| 157752   | -              | Oxy     | ketone    | 574 | 1.08 | 69 | 850 | 851 | 933 | 841 |
| Ethylbenzene             | 100-41-4| 158822    | G2B            | HC      | monocyclic aromatic HC | 600 | 0.46 | 91 | 862 | 862 | 912 | 881 |
| 2-Furanmethanol          | 98-00-0 | 463642    | G2B            | Het     | furan     | 600 | 0.64 | 98 | 862 | 859 | 932 | 830 |
| Pyridine, 3-methyl-      | 108-99-6| 2815906   | M              | Het     | pyridine  | 600 | 0.77 | 93 | 862 | 861 | 953 | 953 |
| 2-Propanone, 1-(acetyloxy)- (2E,4E)-2,4-Hexadienal | 592-20-1 | 4938899 | - | Oxy | ester | 610 | 1.49 | 43 | 867 | 867 | 964 | 944 |
| m-Xylene                | 108-38-3 | 484063   | G3             | HC      | monocyclic aromatic HC | 620 | 0.47 | 91 | 871 | 871 | 942 | 933 |

Continued on next page
| Tentative Identification | CAS    | Peak Area | Health Effects | Class | Subclass | 1<sub>IR</sub> (s) | 2<sub>IR</sub> (s) | Quant Mass | Exp. RI<sup>+</sup> | Lib. RI<sup>+</sup> | Reverse<sup>†</sup> | Similarity<sup>‡</sup> |
|--------------------------|--------|-----------|----------------|-------|----------|-----------------|----------------|------------|-----------------|-----------------|-----------------|-----------------|
| o-Xylene                 | 95-47-6 | 118989    | G3             | HC    | monocyclic aromatic HC | 624             | 0.46          | 91           | 873             | 874             | 928             | 802             |
| Pyridine, 2,6-dimethyl-  | 108-48-5 | 220664    | M              | Het   | pyridine monocyclic aromatic HC | 644             | 0.5           | 107          | 882             | 880             | 961             | 903             |
| Styrene                  | 100-42-5 | 411657    | G2A            | HC    | monocyclic aromatic HC | 668             | 0.5           | 104          | 894             | 894             | 958             | 920             |
| p-Xylene                 | 106-42-3 | 207834    | G3             | HC    | monocyclic aromatic HC | 670             | 0.49          | 91           | 895             | 894             | 942             | 918             |
| Cyclohexanone            | 108-94-1 | 154507    | G3             | Oxy   | ketone  | 674             | 1.04          | 55           | 897             | 895             | 911             | 812             |
| Pyridine, 2-ethyl-       | 100-71-0 | 410300    | -              | Het   | pyridine | 690             | 0.55          | 106          | 904             | 904             | 928             | 918             |
| 2-Cyclopenten-1-one, 2-methyl- | 1120-73-6 | 3068641   | -              | Oxy   | ketone  | 694             | 1.01          | 67           | 906             | 907             | 971             | 970             |
| Pyrazine, 2,6-dimethyl-  | 1192-62-7 | 1507214   | M              | Het   | pyrazine | 710             | 0.6           | 108          | 913             | 912             | 948             | 943             |
| 2-acetylfuran            | 108-50-9 | 985256    | M              | Het   | furan   | 710             | 1.04          | 95           | 913             | 914             | 923             | 892             |
| Pyrazine, ethyl-         | 13925-00-3 | 200279    | M              | Het   | pyrazine | 720             | 0.61          | 107          | 918             | 917             | 928             | 855             |
| Pyrazine, 2,3-dimethyl-  | 5910-89-4 | 388943    | X              | Het   | pyrazine | 724             | 0.61          | 67           | 920             | 920             | 873             | 839             |
| Pyridine, 2,4-dimethyl-  | 108-47-4 | 449871    | M              | Het   | pyridine | 752             | 0.62          | 106          | 932             | 932             | 955             | 925             |
| 2-Cyclohex-1-one         | 930-68-7 | 463075    | M              | Oxy   | ketone  | 758             | 1.14          | 68           | 935             | 939             | 924             | 863             |
| Pyridine, 2,5-dimethyl-  | 589-93-5 | 181366    | -              | Het   | pyridine | 760             | 0.615         | 106          | 936             | 946             | 834             | 791             |
| Pyridine, 2,3-dimethyl-  | 583-61-9 | 232018    | M              | Het   | pyridine monocyclic aromatic HC | 780             | 0.64          | 106          | 945             | 945             | 930             | 886             |
| Benzene, 2-propenyl-     | 300-57-2 | 36610     | X              | HC    | monocyclic aromatic HC | 786             | 0.45          | 117          | 948             | 947             | 925             | 832             |
| 2-Heptanone, 6-methyl-   | 928-68-7 | 259963    | -              | Oxy   | ketone  | 802             | 0.83          | 43           | 955             | 956             | 897             | 777             |
| Benzene, propyl-         | 103-65-1 | 266447    | -              | HC    | monocyclic aromatic HC | 804             | 0.44          | 91           | 956             | 956             | 954             | 899             |
| Cyclopentanone, 3,4-bis(methylene)- | 27646-73-7 | 165346    | -              | Oxy   | ketone  | 810             | 0.88          | 79           | 959             | 949             | 880             | 773             |
Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification            | CAS      | Peak Area | Health Effects | Class       | Subclass       | $t_R$ (s) | $2t_R$ (s) | Mass        | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|------------------------------------|----------|-----------|----------------|-------------|----------------|-----------|------------|-------------|----------|----------|----------|-------------|
| Pyridine, 3-ethyl-                 | 536-78-7 | 646085    | -              | Het         | pyridine       | 814       | 0.72       | 92          | 961      | 962      | 961      | 953         |
| 3-Ethylcyclopentanone              | 10264-55-8 | 126601    | -              | Oxy         | ketone         | 816       | 0.995      | 83          | 962      | 965      | 941      | 884         |
| Benzene, 1-ethyl-2-methyl-         | 611-14-3 | 487535    | -              | HC          | monocyclic aromatic HC | 820       | 0.44       | 105         | 964      | 965      | 921      | 920         |
| Pentanoic acid, 3-methyl-          | 105-43-1 | 617905    | -              | Oxy         | carboxylic acid | 824       | 0.515      | 60          | 965      | 968      | 929      | 826         |
| 2-Butanone, 1-(acetyloxy)-         | 1575-57-1 | 519029    | -              | Oxy         | ketone         | 824       | 1.17       | 57          | 966      | 969      | 874      | 816         |
| Benzaldehyde                       | 100-52-7 | 293884    | M              | Oxy         | aldehyde       | 826       | 0.84       | 106         | 966      | 968      | 937      | 890         |
| 3-Methyl-2-cyclopent-1-one         | 2758-18-1 | 1796553   | -              | Oxy         | ketone         | 826       | 1.38       | 96          | 967      | 969      | 945      | 943         |
| 2-Furancarboxaldehyde, 5-methyl-   | 620-02-0 | 582178    | M              | Het         | furan          | 828       | 1.07       | 110         | 967      | 969      | 951      | 887         |
| Pyridine, 3-ethenyl-               | 1121-55-7 | 2424660   | -              | Het         | pyridine       | 836       | 0.69       | 105         | 971      | 972      | 936      | 933         |
| Benzene, 1,2,4-trimethyl-          | 95-63-6  | 233187    | M              | HC          | monocyclic aromatic HC | 838       | 0.44       | 105         | 972      | 976      | 942      | 931         |
| 1,3-Dimethyltrisulfane             | 3658-80-8 | 50862     | Misc           | Misc        | trisulfide     | 840       | 0.49       | 126         | 973      | 976      | 935      | 828         |
| 2-Methyl-6-methylene-1,7-octadiene | 1686-30-2 | 61641    | -              | HC          | alkene         | 852       | 0.375      | 79          | 978      | 981      | 885      | 784         |
| 3-Methyl-2(5H)-furanone            | 22122-36-7 | 216625    | -              | Oxy         | ketone         | 856       | 1.73       | 98          | 981      | 982      | 914      | 763         |
| Benzene, 1-ethyl-4-methyl-         | 622-96-8 | 70791     | -              | HC          | monocyclic aromatic HC | 858       | 0.46       | 120         | 981      | 977      | 969      | 919         |
| Benzene, (1-methylthenehy)-        | 98-83-9  | 44377     | G2B            | HC          | monocyclic aromatic HC | 864       | 0.47       | 118         | 984      | 986      | 918      | 846         |
| Pyridine, 3,4-dimethyl-            | 583-58-4 | 76132     | -              | Het         | pyridine       | 864       | 0.79       | 107         | 984      | 986      | 914      | 794         |
| 5-Hepten-2-one, 6-methyl-          | 110-93-0 | 565929    | -              | Oxy         | ketone         | 868       | 0.77       | 43          | 986      | 986      | 929      | 897         |
| Phenol                             | 108-95-2 | 14254161  | G3             | Oxy         | alcohol        | 870       | 0.49       | 94          | 986      | 987      | 965      | 963         |
| Benzonitrile                       | 100-47-0 | 1356953   | M              | Nit         | nitrile        | 876       | 1.02       | 103         | 989      | 987      | 952      | 941         |
| beta-Myrcene                       | 123-35-3 | 351424    | G2B            | HC          | monoterpene    | 878       | 0.36       | 69          | 990      | 990      | 909      | 891         |

Continued on next page
Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification                     | CAS     | Peak Area | Health Effects | Class | Subclass      | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI$^*$ | Lib. RI$^*$ | Reverse$^1$ | Similarity$^2$ |
|-----------------------------------------------|---------|-----------|----------------|-------|---------------|-----------|-----------|------------|------------|-------------|-------------|----------------|
| Pyridine, 2,4,6-trimethyl-                    | 111-13-7| 98961     | -              | Het   | pyridine      | 880       | 0.495     | 121        | 991        | 993         | 865         | 808            |
| 2-Octanone                                    | 108-75-8| 176216    | -              | Oxy   | ketone        | 880       | 0.8       | 58         | 991        | 991         | 861         | 776            |
| 1,2,3-Trimethylcyclohexane                    | 1678-81-5| 199774    | -              | HC    | alicyclic HC  | 882       | 0.315     | 69         | 992        | NA          | 840         | 817            |
| Cyclopropene, 3-(1-methylethenyl)-1-(1-     | NA      | 76431     | -              | HC    | alicyclic HC  | 884       | 0.435     | 91         | 993        | NA          | 934         | 766            |
| methylethyl)-1-(1-methylethyl)-              |         |           |                |       |               |           |           |            |            |             |             |                |
| 2-Cyclopenten-1-one, 3,4-dimethyl-            | 30434-64-1 | 939188 | -              | Oxy   | ketone        | 886       | 1.21      | 95         | 994        | 986         | 885         | 890            |
| Pyridine, 2-propyl-                           | 622-39-9| 217828    | -              | Het   | pyridine      | 890       | 0.51      | 93         | 996        | 998         | 912         | 784            |
| Benzene, 1-ethenyl-3-methyl-                  | 100-80-1| 414045    | G3             | HC    | monocyclic    | 894       | 0.49      | 117        | 997        | 991         | 769         | 854            |
| 2-Cyclohexen-1-one, 6-(1-hydroxy-1-methylethyl)-3-methyl- | 37902-41-3 | 275954 | -              | Oxy   | ketone        | 894       | 0.87      | 82         | 998        | NA          | 749         | 770            |
| 5-Hydroxy-2-heptanone                         | NA      | 1280604   | -              | Oxy   | ketone        | 894       | 0.9       | 67         | 998        | NA          | 924         | 890            |
| 1,5-Heptadiene, 2,3,6-trimethyl-              | 33501-88-1 | 322460 | -              | HC    | alkene        | 896       | 0.315     | 69         | 998        | NA          | 904         | 879            |
| Pyrazine, 2-ethyl-6-methyl-                   | 13925-03-6 | 408895 | -              | Het   | pyrazine      | 896       | 0.53      | 121        | 998        | 998         | 914         | 906            |
| Benzofuran                                    | 271-89-6| 138824    | -              | Het   | furan         | 898       | 0.54      | 90         | 999        | 1000        | 879         | 850            |
| Decane                                        | 5584-69-0 | 99700    | -              | HC    | alkane        | 900       | 0.31      | 57         | 1000       | 1000        | 924         | 870            |
| 2-Furanone, 2,5-dihydro-3,5-dimethyl          | 124-18-5| 431799    | X              | Het   | furan         | 900       | 1.73      | 69         | 1001       | 993         | 874         | 847            |
| Benzene, 1-ethenyl-4-methyl-                  | 622-97-9 | 90145     | -              | HC    | monocyclic    | 906       | 0.48      | 118        | 1003       | 995         | 754         | 840            |
| Pyrazine, trimethyl-                          | 14667-55-1 | 1430567 | -              | Het   | pyrazine      | 906       | 0.51      | 42         | 1003       | 1002        | 975         | 917            |
| Pyrazine, 2-ethyl-3-methyl-                   | 15707-23-0 | 109963 | -              | Het   | pyrazine      | 906       | 0.52      | 121        | 1003       | 1003        | 836         | 827            |
| Butanamide, 3-methyl-                         | 541-46-8 | 624114    | -              | Nit   | amide         | 912       | 1.15      | 59         | 1006       | NA          | 909         | 799            |
| Pyridine, 2,3,6-trimethyl-                    | 1462-84-6 | 97524    | -              | Het   | pyridine      | 914       | 0.48      | 120        | 1007       | 1009        | 873         | 847            |

*Continued on next page*
| Tentative Identification                          | CAS       | Peak Area | Health Effects | Class       | Subclass | 1\text{TR} (s) | 2\text{TR} (s) | Quant | Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|------------------------------------------------|-----------|-----------|----------------|-------------|----------|----------------|----------------|-------|------|---------|---------|---------|------------|
| 2-Hydroxy-gamma-butyrolactone                    | 19444-84-9 | 1653501   | -              | Oxy lactone | -        | 916            | 1.325          | 57    | 1008 | NA      | 904     | 873     |
| 1-Pyrrolidinylacetonitrile                       | 29134-29-0 | 222313    | X              | Het         | pyridine  | 920            | 0.92           | 82    | 1010 | NA      | 945     | 935     |
| 1-Propanone, 1-(2-furanyl)-                      | 3194-15-8  | 186103    | -              | Het         | furan     | 922            | 0.84           | 95    | 1011 | 1011    | 947     | 761     |
| 3-Pyridine carbonitrile                          | 100-54-9   | 445395    | X              | Het         | pyridine  | 926            | 1.12           | 104   | 1013 | 1012    | 958     | 864     |
| 1-Decene, 4-methyl-                              | 13151-29-6 | 50017     | -              | HC alkene   | -        | 930            | 0.325          | 57    | 1015 | NA      | 854     | 753     |
| 5,6,7,8-Tetrahydroindolizine                     | 13618-88-7 | 259913    | -              | Nit aza-arene | -        | 930            | 0.535          | 120   | 1015 | NA      | 809     | 843     |
| Glycerin                                        | 56-81-5    | 72303956  | M              | Oxy alcohol | -        | 932            | 0.685          | 61    | 1016 | NA      | 922     | 920     |
| N,3-Dimethylaniline                              | 696-44-6   | 463788    | -              | Nit amine   | -        | 938            | 0.525          | 120   | 1019 | NA      | 777     | 822     |
| gamma-Terpinene                                 | 99-85-4    | 25541     | M              | HC monoterpenes | -        | 940            | 0.36           | 93    | 1020 | 1024    | 753     | 860     |
| p-Methylanisole                                  | 22748-16-9 | 159767    | -              | Oxy ether   | -        | 948            | 0.52           | 122   | 1024 | 1024    | 922     | 894     |
| 4,4-Dimethyl-2-cyclopentene-1-one                | 104-93-8   | 542221    | X              | Oxy ketone  | -        | 948            | 1.34           | 95    | 1024 | NA      | 884     | 874     |
| Benzene, 1,2,3-trimethyl-                         | 526-73-8   | 858011    | M              | HC monocyclic aromatic HC | -        | 950            | 0.47           | 105   | 1025 | 1028    | 925     | 926     |
| 4-Isopropylpyridine                              | 5749-72-4  | 101837    | -              | Het         | pyridine  | 952            | 0.7            | 106   | 1026 | 1021    | 864     | 760     |
| Cyclohexane, (1-methylethylidene)-               | 696-30-0   | 225112    | -              | HC alicyclic HC | -        | 952            | 0.78           | 81    | 1026 | NA      | 822     | 783     |
| Cyclohexene, 3-methyl-6-(1-methylethyl)-         | 5256-65-5  | 526209    | -              | HC alicyclic HC | -        | 954            | 0.35           | 67    | 1026 | NA      | 917     | 916     |
| o-Cymene                                        | 56613-80-0 | 675476    | -              | HC monocyclic aromatic HC | -        | 956            | 0.39           | 119   | 1027 | 1027    | 946     | 937     |
| d(-)-á-Phenylglycinol                            | 765-70-8   | 237249    | -              | Oxy alcohol | -        | 956            | 0.56           | 106   | 1028 | NA      | 808     | 853     |
| 1,2-Cyclopentanedione, 3-methyl-                 | 527-84-4   | 3253642   | -              | Oxy ketone  | -        | 956            | 0.835          | 112   | 1028 | NA      | 963     | 959     |
| Spiro[2,4]heptan-5-one                           | 19740-31-9 | 134988    | -              | Oxy ketone  | -        | 960            | 0.94           | 110   | 1030 | NA      | 855     | 841     |
| 1-Hexanol 2-ethyl-                               | 104-76-7   | 1229495   | M              | Oxy alcohol | -        | 962            | 0.465          | 57    | 1030 | 1030    | 953     | 905     |

Continued on next page
| Tentative Identification                  | CAS      | Peak Area | Health Effects | Class          | Subclass         | $t_R$ (s) | $2^{t_R}$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse $\dagger$ | Similarity $\ddagger$ |
|------------------------------------------|----------|-----------|----------------|----------------|------------------|-----------|-------------|------------|--------|--------|-------------------|----------------------|
| Benzene, cyclopropyl-                    | 873-49-4 | 703538    | M              | HC             | monocyclic       | 962       | 0.48        | 117        | 1030   | 1032   | 919               | 945                  |
| D-Limonene                               | 5989-27-5| 4202273   | G3             | HC             | monoterpene      | 966       | 0.35        | 68         | 1032   | NA     | 949               | 948                  |
| Pyridine, 3-ethyl-4-methyl-1-Methylcyclooctene | 933-11-9 | 69006     | M              | Het            | pyridine         | 968       | 0.59        | 106        | 1033   | 1033   | 854               | 768                  |
| 1,3,5-Cycloheptatriene, 7,7-dimethyl-    | 529-21-5 | 355142    | -              | HC             | alkene           | 968       | 0.795       | 96         | 1033   | 1023   | 835               | 820                  |
| 1,2,4-Cyclohexatriene, 7,7-dimethyl-     | 1122-62-9| 74150     | M              | HC             | alicyclic        | 974       | 0.49        | 105        | 1036   | NA     | 846               | 777                  |
| 1-(2-Pyridinyl)ethane                    | 05/07/7533 | 232753    | -              | Het            | pyridine         | 974       | 0.74        | 79         | 1036   | 1036   | 920               | 875                  |
| trans-beta-Ocimene                       | 1193-79-9 | 256261    | -              | HC             | monoterpene      | 976       | 0.34        | 93         | 1037   | 1037   | 874               | 885                  |
| 2-Acetyl-5-methylfuran                   | 1121-05-7 | 128502    | -              | Het            | furan            | 976       | 1           | 124        | 1037   | 1037   | 896               | 867                  |
| 2-Cyclopenten-1-one, 2,3-dimethyl-       | 13877-91-3 | 5811666  | -              | Oxy            | ketone           | 976       | 1.08        | 67         | 1037   | 1036   | 892               | 893                  |
| Benzene, 1-ethenyl-2-methyl-             | 611-15-4 | 399199    | M              | HC             | monocyclic       | 980       | 0.45        | 117        | 1039   | NA     | 845               | 821                  |
| Cyclopentanone, 2-ethyl-                 | 4971-18-0 | 123467    | -              | Oxy            | ketone           | 980       | 0.81        | 84         | 1039   | NA     | 859               | 776                  |
| 3,4,5,6-Tetrahydropthalic anhydride       | 2426-02-0 | 280177    | -              | Oxy            | anhydride        | 982       | 1.03        | 79         | 1040   | NA     | 857               | 792                  |
| (3E)-3,7-Dimethyl-1,3,7-octatriene       | 100-51-6  | 124778    | M              | HC             | alkene           | 986       | 0.345       | 93         | 1042   | 1042   | 882               | 842                  |
| Benzyl alcohol                           | 502-99-8  | 210470    | -              | Oxy            | alcohol          | 986       | 0.58        | 79         | 1042   | 1041   | 930               | 896                  |
| Pyridine, 5-ethenyl-2-methyl-            | 872-50-4  | 130749    | M              | Het            | pyridine         | 988       | 0.675       | 118        | 1043   | 1040   | 756               | 791                  |
| 2-Pyrrolidinone, 1-methyl-               | 140-76-1  | 103660    | X              | Het            | pyrrole          | 988       | 1.55        | 99         | 1044   | 1045   | 946               | 769                  |
| Benzene, 3-butenyl-                      | 768-56-9  | 199958    | -              | HC             | monocyclic       | 994       | 0.42        | 91         | 1046   | 1038   | 888               | 841                  |
| Pyridine, 2-(2-methylpropyl)-            | 6304-24-1 | 181614    | -              | Het            | pyridine         | 996       | 0.49        | 93         | 1047   | NA     | 878               | 848                  |
| (3E)-3,7-Dimethyl-1,3,6-octatriene       | 3779-61-1 | 341126    | -              | HC             | alkene           | 998       | 0.345       | 93         | 1048   | NA     | 926               | 910                  |
| Tentative Identification                  | CAS     | Peak Area | Health Effects | Class | Subclass          | \( t_1 \) (s) | \( t_2 \) (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|------------------------------------------|---------|-----------|----------------|-------|-------------------|---------------|---------------|-------------|---------|---------|---------|------------|
| 3-Hydroxy-4,4-dimethylidihydro-2(3H)-furanone | 52126-90-6 | 425299    | -              | Oxy   | Ketone            | 998           | 1.265         | 71          | 1048    | NA      | 942     | 916        |
| Indene                                   | 95-13-6 | 1195501   | -              | HC    | Polycyclic aromatic HC | 1000           | 0.51          | 116         | 1049    | 1049    | 928     | 928        |
| 1,2-Diethylbenzene                       | 135-01-3 | 42400     | M              | HC    | Monocyclic aromatic HC | 1002           | 0.4           | 119         | 1050    | 1048    | 794     | 754        |
| Benzene, 1-methyl-3-propyl-              | 1074-43-7 | 312320    | -              | HC    | Monocyclic aromatic HC | 1010           | 0.4           | 105         | 1054    | 1054    | 846     | 883        |
| Pyridine 3-propyl-                       | 4673-31-8 | 444053    | -              | Het   | Pyridine          | 1014           | 0.675         | 92          | 1056    | NA      | 876     | 865        |
| 2-Tolyloxirane                           | 2783-26-8 | 287737    | -              | Oxy   | Epoxide           | 1020           | 0.4           | 105         | 1058    | NA      | 866     | 861        |
| Pyridine, 3-ethyl-5-methyl-              | 1193-18-6 | 84660     | -              | Het   | Pyridine          | 1020           | 0.6           | 121         | 1059    | NA      | 797     | 845        |
| 2-Cyclohexen-1-one, 3-methyl-            | 3999-78-8 | 315740    | -              | Oxy   | Ketone            | 1020           | 1.205         | 82          | 1059    | NA      | 954     | 897        |
| Acetic acid, phenyl ester                | 122-79-2 | 370084    | -              | Oxy   | Esters            | 1022           | 0.83          | 94          | 1060    | 1065    | 955     | 924        |
| Phenol, 2-methyl-                        | 95-48-7  | 3522348   | G3             | Oxy   | Alcohol           | 1024           | 0.49          | 108         | 1060    | 1060    | 951     | 950        |
| 2-Cyclopenten-1-one, 2,3,4-trimethyl-    | 28790-86-5 | 982342    | -              | Oxy   | Ketone            | 1026           | 0.94          | 109         | 1062    | 1063    | 896     | 879        |
| Pyridine, 2-ethyl-4,6-dimethyl-           | 1124-35-2 | 103131    | -              | Het   | Pyridine          | 1038           | 0.425         | 134         | 1067    | 1080    | 797     | 767        |
| Benzene, 1-methyl-2-propyl-              | 3658-77-3 | 254982    | M              | HC    | Monocyclic aromatic HC | 1040           | 0.44          | 105         | 1068    | 1067    | 901     | 887        |
| 2,5-Dimethyl-4-hydroxy-3(2H)-furanone     | 1074-17-5 | 193748    | -              | Het   | Furan             | 1040           | 0.675         | 57          | 1068    | 1068    | 927     | 811        |
| Pyridine, 2,3,5-trimethyl-                | 695-98-7  | 70191     | -              | Het   | Pyridine          | 1042           | 0.61          | 121         | 1069    | 1076    | 894     | 806        |
| 2-Acetylpyrrole                          | 98-86-2  | 533682    | M              | Het   | Pyrrole           | 1044           | 0.78          | 94          | 1070    | 1072    | 907     | 926        |
| Acetophenone                             | 1072-83-9 | 1246782   | M              | Oxy   | Ketone            | 1044           | 0.84          | 105         | 1070    | 1070    | 974     | 972        |
Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification | CAS     | Peak Area | Health Effects | Class            | Subclass | $t_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|--------------------------|---------|-----------|----------------|------------------|----------|----------|-----------|--------|--------|---------|------------|
| 3-Methylbenzaldehyde     | 620-23-5| 318144    | -              | Oxy              | aldehyde | 1046     | 0.91      | 90     | 1071   | NA      | 952        |
| 2-Ethyl-3,5-dimethylpyridine | 1123-96-2| 40278    | -              | Het              | pyridine | 1048     | 0.415     | 134    | 1072   | NA      | 863        |
| Pyridine, 5-ethyl-2-methyl- | 104-90-5| 66317     | M              | Het              | pyridine | 1054     | 0.705     | 106    | 1075   | NA      | 887        |
| Benzaldehyde, 2-methyl-   | 529-20-4| 160338    | -              | Oxy              | aldehyde | 1054     | 0.79      | 91     | 1075   | 1068    | 814        |
| Pyrazine, 3-ethyl-2,5-dimethyl- | 21834-98-0| 99952  | -              | Het              | pyrazine | 1058     | 0.46      | 136    | 1077   | 1077    | 885        |
| 2-Hydroxy-3,5-dimethylcyclopent-2-en-1-one | 5682-69-9| 122759   | -              | Oxy              | ketone   | 1058     | 0.825     | 111    | 1077   | NA      | 780        |
| 2-Cyclopenten-1-one, 3-ethyl- | 13360-65-1| 1045353 | -              | Oxy              | ketone   | 1058     | 1.23      | 81     | 1077   | 1071    | 910        |
| Benzene, 2-ethyl-1,4-dimethyl- | 1758-88-9| 174002   | -              | HC               | monocyclic aromatic HC | 1060 | 0.42 | 119 | 1078 | 1077 | 926 | 906 |
| Benzene, 1-ethyl-2,4-dimethyl- | 616-45-5| 391304    | M              | HC               | monocyclic aromatic HC | 1066 | 0.405 | 119 | 1081 | 1080 | 906 | 910 |
| Octanenitrile            | 124-12-9| 64009     | -              | Nit              | nitrile  | 1066     | 0.97      | 82     | 1081   | 1082    | 887        |
| 2-Pyrrolidinone          | 874-41-9| 962149    | X              | Het              | pyrrole  | 1066     | 1.44      | 85     | 1081   | 1078    | 929        |
| p-Cresol                 | 106-44-5| 9677027   | M              | Oxy              | alcohol  | 1068     | 0.48      | 107    | 1082   | 1082    | 950        |
| Pyrazine, 2-ethyl-3,5-dimethyl-1,10-Undecadiene | 13925-07-0| 118710 | -              | Het              | pyrazine | 1070     | 0.455     | 135    | 1083   | 1083    | 830        |
| 5-Ethyl-2,3-dimethylpyrazine | 13688-67-0| 40492    | -              | HC               | alkene   | 1072     | 0.33      | 67     | 1084   | 1085    | 870        |
| Benzene, 1-methyl-1,2-propadienyl- | 22433-39-2| 97513    | -              | Het              | pyrazine | 1076     | 0.465     | 135    | 1086   | 1087    | 962        |
| Benzene, 1-methyl-3-(1-methylethyl)- | 15707-34-3| 134797   | -              | HC               | monocyclic aromatic HC | 1076 | 0.48 | 115 | 1086 | NA | 832 | 847 |
| Benzene, 1-methyl-3-(1-methylethyl)-2,3-Dihydro-5-hydroxy-6-methyl-4H-pyran-4-one | 535-77-3| 1207247   | X              | Het              | pyran    | 1078     | 0.775     | 43     | 1087   | 1088    | 974        |

Continued on next page
| Tentative Identification | CAS | Peak Area | Health Effects | Class | Subclass | \( t_R (s) \) & \( t_R (s) \) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|-------------------------|-----|-----------|----------------|-------|----------|--------|---------|-------|--------|---------|-----------|
| 1,5-Heptadiene, 2,5-dimethyl-3-methylene- | 90-05-1 | 178834 | G2B | HC | alkene | 1082 & 0.325 | 93 | 1089 | NA | 892 | 877 |
| 1H-Indene, 2,3-dihydromethyl- | 7251-61-8 | 63330 | M | HC | polycyclic aromatic HC | 1082 & 0.43 | 132 | 1089 | 1087 | 919 | 873 |
| Guaiacol | 620-22-4 | 3446021 | - | Oxy | alcohol | 1082 & 0.67 | 109 | 1089 | 1089 | 937 | 933 |
| 3-Methylbenzonitrile | 27133-93-3 | 93252 | - | Nit | nitrile | 1082 & 0.81 | 91 | 1089 | 1086 | 910 | 796 |
| 2-Nonanone | 81396-36-3 | 252097 | - | Oxy | ketone | 1086 & 0.72 | 58 | 1091 | 1091 | 918 | 859 |
| 1-Undecene | 821-55-6 | 294508 | - | HC | alkene | 1088 & 0.32 | 56 | 1091 | 1091 | 928 | 928 |
| 2,5-Pyrrolidinedione, 1-methyl- | 1121-07-9 | 251451 | X | Het | pyrrole | 1088 & 1.505 | 113 | 1092 | NA | 951 | 891 |
| 4,5-Dimethyl-4-hexen-3-one | 17325-90-5 | 210882 | - | Oxy | ketone | 1092 & 1.49 | 97 | 1094 | NA | 921 | 794 |
| Benzonitrile, 2-methyl- | 529-19-1 | 354574 | X | Nit | nitrile | 1094 & 0.98 | 116 | 1095 | NA | 941 | 927 |
| 3-Undecene, (Z)- | 821-95-4 | 37958 | - | HC | alkene | 1098 & 0.305 | 69 | 1096 | 1092 | 754 | 844 |
| Undecane | 23074-10-4 | 491737 | - | HC | alkane | 1104 & 0.29 | 57 | 1099 | 1100 | 952 | 933 |
| 5-Ethyl-2-furaldehyde | 1120-21-4 | 240551 | X | Het | furan | 1104 & 1.09 | 109 | 1100 | NA | 850 | 812 |
| Benzo[1,2-c]furan, 7-methyl- | 17059-52-8 | 129716 | - | Het | furan | 1106 & 0.505 | 131 | 1100 | NA | 850 | 863 |
| 3-Ethenyl-3-methylcyclopentanone | 49664-66-6 | 981873 | - | Oxy | ketone | 1108 & 1.11 | 68 | 1102 | NA | 770 | 773 |
| Benzene, 1-methyl-4-(2-methylpropyl)- | 06/04/5161 | 248723 | - | HC | monocyclic aromatic HC | 1110 & 0.395 | 105 | 1102 | 1105 | 882 | 873 |
| 2-Methyl-6-propylpyridine | 5397-28-4 | 183484 | - | Het | pyridine | 1110 & 0.495 | 107 | 1102 | NA | 824 | 779 |
| 1,3-Dimethyl-2-vinylbenzene | 24081-57-0 | 48068 | - | HC | monocyclic aromatic HC | 1112 & 0.44 | 132 | 1103 | NA | 865 | 787 |
| 1-(1,5-Dimethylbicyclo[2.1.0]pent-5-yl)ethanone | 218-029-4 | 114146 | - | Oxy | ketone | 1112 & 0.835 | 95 | 1104 | NA | 793 | 753 |
| 2-Undecene, (E)- | 693-61-8 | 44179 | X | HC | alkene | 1114 & 0.3 | 70 | 1104 | 1104 | 863 | 899 |
### Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification | CAS     | Peak Area | Health Effects | Class       | Subclass          | $^{1}t_{R} (s)$ | $^{2}t_{R} (s)$ | Quant Mass | Exp. RI | Lib. RI | Reverse $^1$ | Similarity $^1$ |
|--------------------------|---------|-----------|----------------|-------------|-------------------|----------------|----------------|------------|---------|---------|--------------|----------------|
| Benzene, 2-ethyl-1,3-dimethyl- | 04/04/2870 | 158420   | -              | HC          | monocyclic aromatic HC | 1118    | 0.43           | 119        | 1107    | 1105   | 775          | 860            |
| 2,6-Diethylpyridine      | 6940-57-4 | 28221     | -              | Het         | pyridine         | 1118    | 0.505          | 135        | 1107    | NA     | 872          | 759            |
| 2-Acetyl-6-methylpyridine | 93518-56-0 | 63460   | -              | Het         | pyridine         | 1118    | 0.675          | 93         | 1107    | 1107   | 853          | 790            |
| 2,3-Dimethylanisole      | 1575-46-8 | 46805     | -              | Oxy         | ether            | 1122    | 0.45           | 121        | 1109    | 1111   | 866          | 801            |
| Benzonitrile, 4-methyl-   | 2944-49-2 | 283505   | -              | Nit         | nitrile          | 1122    | 1              | 117        | 1109    | NA     | 929          | 896            |
| 2,3-Dimethyl-4-hydroxy-2- | 104-85-8 | 307761   | X              | Oxy         | ester            | 1122    | 1.88           | 55         | 1110    | NA     | 920          | 843            |
| butenoic lactone         | 6,7-Dihydro-5H-cyclopentapyrazine | 626-97-1 | 87336         | -          | Het              | 1124    | 0.61           | 119        | 1110    | 1104   | 948          | 818            |
| Pentanamide              | NA      | 534540    | -              | Nit         | amide            | 1124    | 1.045          | 59         | 1110    | NA     | 765          | 854            |
| Phenol, 2,6-dimethyl-     | 74744-54-0 | 642988   | -              | Oxy         | alcohol          | 1126    | 0.5            | 107        | 1111    | 1108   | 945          | 933            |
| 2-Acetyl-4-methylthiazole| 576-26-1 | 30286     | X              | Nit         | thiazole         | 1126    | 0.64           | 113        | 1111    | 1118   | 950          | 807            |
| Benzo[4,5]furan, 2-methyl- | 4265-25-2 | 609985   | -              | Het         | furan            | 1128    | 0.53           | 131        | 1112    | 1117   | 930          | 924            |
| Cyclohexane, 1-methyl-4-(1- | 350-03-8 | 60114     | M              | HC          | monoterpene      | 1130    | 0.725          | 95         | 1113    | NA     | 838          | 789            |
| methylthylidene)-        |         |           |                |             |                  |         |                |            |         |        |              |                |
| 1-(3-Pyridinyl)ethanone   | 1124-27-2 | 577365   | -              | Het         | pyridine         | 1130    | 1.02           | 78         | 1113    | 1117   | 928          | 887            |
| (E)-4,8-Dimethyl[1,3,7]-  | 19945-61-0 | 337089  | -              | HC          | alicyclic HC     | 1132    | 0.34           | 69         | 1114    | 1114   | 883          | 855            |
| triene                   |         |           |                |             |                  |         |                |            |         |        |              |                |
| 2,3-Cyclopentenopyridine | 533-37-9 | 365157    | -              | Het         | pyridine         | 1132    | 0.66           | 118        | 1114    | NA     | 873          | 821            |
| Benzeno[1,2-a]pyridine    | 118-71-8 | 236537   | M              | Oxy         | ether            | 1136    | 0.47           | 121        | 1116    | 1122   | 929          | 901            |
| 1H-Indole, 2,3-dihydro-   | 496-15-1 | 123433    | -              | Nit         | aza-arene        | 1136    | 0.58           | 118        | 1116    | NA     | 871          | 831            |
| Maltol                   | 1515-95-3 | 822603   | -              | Oxy         | alcohol          | 1136    | 0.91           | 126        | 1116    | 1122   | 926          | 916            |
| 2-Acetyl-3-methylpyrazine | 54458-61-6 | 85387   | -              | Het         | pyrazine         | 1138    | 0.78           | 94         | 1118    | 1128   | 810          | 752            |
| 2-Cyclopenten-1-one,      | 23787-80-6 | 206877  | -              | Oxy         | ketone           | 1138    | 0.835          | 123        | 1118    | NA     | 858          | 846            |
| 2,3,4,5-tetramethyl-      |         |           |                |             |                  |         |                |            |         |        |              |                |
| 3-Pyridinyl acetate       | 17747-43-2 | 215416  | -              | Het         | pyridine         | 1138    | 1.015          | 95         | 1118    | 1127   | 899          | 784            |

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| Tentative Identification | CAS         | Peak Area  | Health Effects | Class         | Subclass      | $^{1}_{t_R}$ (s) | $^{2}_{t_R}$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|--------------------------|-------------|------------|----------------|---------------|---------------|-----------------|-----------------|-------------|----------|----------|----------|------------|
| Bicyclo[5.1.0]octane, 8-(1-methylethylidene)- | 54166-47-1  | 106957     | -              | HC            | polycyclic aromatic HC | 1140            | 0.325           | 93          | 1118     | NA       | 829       | 791        |
| Benzeneneethanol         | 60-12-8     | 323888     | X              | Oxy           | alcohol        | 1140            | 0.58            | 92          | 1118     | 1117     | 931       | 899        |
| Benzene, 1,2,4,5-tetramethyl- | 622-80-0   | 143148     | -              | HC            | monocyclic aromatic HC | 1142            | 0.41            | 119         | 1119     | 1118     | 857       | 840        |
| N-Phenyl-N-propylamine   | 21835-01-8  | 110715     | -              | Nit           | amine         | 1142            | 0.53            | 106         | 1119     | NA       | 968       | 764        |
| Benoxazole, 2-methyl-     | 95-21-6     | 199375     | -              | Nit           | oxazole       | 1142            | 0.56            | 133         | 1119     | NA       | 910       | 865        |
| 2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- | 95-93-2    | 627333     | X              | Oxy           | ketone        | 1142            | 0.77            | 83          | 1120     | 1121     | 947       | 926        |
| Pentanamide, 4-methyl-    | 1119-29-5   | 646105     | -              | Nit           | amide         | 1146            | 1.08            | 59          | 1122     | NA       | 836       | 886        |
| Benzene, 1,2,3,5-tetramethyl- | 527-53-7   | 368949     | X              | HC            | monocyclic aromatic HC | 1148            | 0.42            | 119         | 1123     | 1123     | 888       | 899        |
| Benzene, (2-methyl-1-propenyl)- | 768-49-0   | 175001     | -              | HC            | monocyclic aromatic HC | 1150            | 0.45            | 117         | 1124     | NA       | 897       | 869        |
| 1-(6-methly-2-pyrazinyl)-1-Ethanone | 22047-26-3 | 58669      | -              | Het           | pyrazine      | 1152            | 0.72            | 136         | 1125     | NA       | 869       | 778        |
| Isophorone               | 78-59-1     | 597876     | X              | Oxy           | ketone        | 1154            | 1.18            | 82          | 1126     | 1126     | 965       | 939        |
| 2H-cyclopenta[b]furan-2-one, 3,3a,6,6a-tetrahydro-, (3aR-cis)- | 43119-28-4 | 185274     | -              | Het           | furan         | 1156            | 1.225           | 96          | 1127     | NA       | 829       | 769        |
| Benzene, 1-butenyl-, (E)- | 1005-64-7   | 456780     | -              | HC            | monocyclic aromatic HC | 1158            | 0.46            | 117         | 1128     | NA       | 946       | 936        |
| 3-Pyridinol              | 109-00-2    | 4853143    | -              | Het           | pyridine      | 1158            | 0.555           | 95          | 1128     | NA       | 934       | 927        |
| Alloocimene              | 3016-19-1   | 292071     | -              | HC            | monoterpenes  | 1160            | 0.37            | 121         | 1129     | 1129     | 915       | 908        |
| Benzyl methyl ketone     | 103-79-7    | 1456828    | -              | Oxy           | ketone        | 1162            | 0.87            | 43          | 1130     | 1124     | 918       | 896        |
| 2-Ethylidenecyclohexanone | 1122-24-3   | 501173     | -              | Oxy           | ketone        | 1162            | 1.01            | 124         | 1130     | NA       | 824       | 879        |

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| Tentative Identification | CAS     | Peak Area | Health Effects | Class     | Subclass             | \( t_R (s) \) | \( 2t_R (s) \) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|--------------------------|---------|-----------|----------------|-----------|----------------------|----------------|---------------|------------|---------|---------|---------|------------|
| Cosmene                  | 460-01-5| 64363     | -              | HC        | monoterpenes         | 1166           | 0.43          | 119        | 1132    | 1132   | 905     | 852       |
| Benzene, 1-methyl-4-(2-propenyl)-| 3333-13-9| 331903     | -              | HC        | aromatic monocyclic | 1170           | 0.455         | 117        | 1134    | NA     | 940     | 920       |
| Benzeneacetaldehyde, α-ethyl-| 2439-43-2| 80968     | -              | Oxy       | aldehyde            | 1176           | 0.385         | 119        | 1137    | NA     | 744     | 767       |
| 3-Pyridinol, 2-methyl-    | 1121-25-1| 435522     | -              | Het       | pyridine           | 1176           | 0.52          | 109        | 1138    | NA     | 938     | 864       |
| Ethanone, 1-(2-methylphenyl)-| 577-16-2| 119774     | -              | Oxy       | ketone             | 1178           | 0.71          | 119        | 1139    | 1139   | 954     | 889       |
| 1-Propanone, 1-(2-pyridinyl)-| 3238-55-9| 87768     | -              | Het       | pyridine           | 1180           | 0.62          | 78         | 1140    | 1137   | 915     | 819       |
| 1-Methylenespiro[2.4]heptan-4-one | 166193-08-4| 167129     | -              | Oxy       | ketone             | 1182           | 0.88          | 79         | 1141    | NA     | 847     | 798       |
| 2-Hepten-4-one, 2-methyl- | 22319-24-0| 147659     | -              | Oxy       | ketone             | 1182           | 1.825         | 83         | 1141    | NA     | 799     | 757       |
| Benzene, 1,3-diethyl-5-methyl- | 140-29-4| 45264     | M              | HC        | monocyclic         | 1184           | 0.365         | 133        | 1142    | 1143   | 837     | 798       |
| (3-methyl-3-butetyl)Benzene | 1619-28-9| 284181     | -              | HC        | monocyclic         | 1184           | 0.405         | 91         | 1142    | NA     | 888     | 804       |
| Benzyl nitrile           | 2050-24-0| 897570     | -              | Nit       | nitrile            | 1184           | 0.98          | 90         | 1142    | 1142   | 941     | 939       |
| 2-Cyclopenten-1-one, 3-(1-methylethyl)- | 6683-51-8| 86044     | -              | Oxy       | ketone             | 1184           | 1.205         | 82         | 1142    | NA     | 916     | 837       |
| 4-Methylindane           | 874-23-7| 481744     | -              | HC        | polycyclic         | 1188           | 0.4          | 117        | 1144    | 1140   | 899     | 909       |
| Cyclohexanone, 2-acetyl- | 821-97-6| 98636     | -              | Oxy       | ketone             | 1188           | 0.695         | 140        | 1144    | NA     | 767     | 753       |
| 2-Ethylhexyl acetate     | 103-09-3| 528671     | X              | Oxy       | ester              | 1192           | 0.555         | 70         | 1146    | 1144   | 923     | 908       |
| 4-Oxoisophorone          | 1125-21-9| 427368     | -              | Oxy       | ketone             | 1194           | 1.095         | 68         | 1147    | 1147   | 905     | 888       |

*Continued on next page*
| Tentative Identification                      | CAS        | Peak Area | Health Effects | Class | Subclass | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|----------------------------------------------|------------|-----------|----------------|-------|----------|-----------|------------|------------|--------|--------|---------|------------|
| 1,3-Hexadiene, 3-ethyl-2,5-dimethyl-         | 62338-07-2 | 177224    | -              | HC    | alkene   | 1196      | 0.89       | 123        | 1148   | NA     | 798     | 810        |
| 2-Isobutyl-4-methylpyridine                  | 85665-88-9 | 552818    | G3             | Het   | pyridine | 1200      | 0.47       | 107        | 1150   | 1154   | 882     | 868        |
| 4H-Pyrano-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- | 28564-83-2 | 1746635   | M              | Het   | pyran    | 1202      | 0.645      | 101        | 1151   | 1151   | 907     | 907        |
| 3-Cyclohexen-1-one, 2,2,5,5-tetramethyl-     | 80933-76-2 | 451997    | -              | Oxy   | ketone   | 1202      | 0.855      | 110        | 1152   | NA     | 839     | 827        |
| 1H-Indene, 1-methyl-                         | 767-59-9   | 456875    | -              | HC    | polycyclic aromatic HC | 1206 | 0.47 | 115 | 1153 | 1149 | 926 | 928 |
| 2-Cyclohexen-1-one, 3,4,4-trimethyl-         | 17299-41-1 | 50433     | -              | Oxy   | ketone   | 1206      | 0.845      | 96         | 1154   | NA     | 860     | 771        |
| Phenol, 2,4-dimethyl-                        | 105-67-9   | 322554    | -              | Oxy   | alcohol  | 1210      | 0.46       | 93         | 1156   | 1156   | 927     | 916        |
| Benzene, (1-methyl-2-cyclopropen-1-yl)-      | 65051-83-4 | 467679    | -              | HC    | monocyclic aromatic HC | 1210 | 0.47 | 130 | 1156 | NA | 928 | 924 |
| Benzene, 1-ethenyl-4-methoxy-               | 637-69-4   | 208631    | -              | Oxy   | ether    | 1214      | 0.53       | 134        | 1158   | 1158   | 880     | 861        |
| Bicyclo[10.1.0]tridec-1-ene                 | 54766-91-5 | 164564    | -              | HC    | polycyclic aromatic HC | 1216 | 0.315 | 67 | 1159 | NA | 786 | 761 |
| Pyridine, 3-butyl-                          | 539-32-2   | 376844    | -              | Het   | pyridine | 1216      | 0.63       | 92         | 1159   | NA     | 928     | 892        |
| Benzene, pentyl-                            | 538-68-1   | 349322    | -              | HC    | monocyclic aromatic HC | 1218 | 0.4 | 92 | 1160 | NA | 940 | 935 |
| Benzene, 1-butynyl-                         | 622-76-4   | 857567    | -              | HC    | monocyclic aromatic HC | 1218 | 0.5 | 129 | 1160 | NA | 928 | 933 |
| 2,5-Pyrrolinedione, 3-methyl-               | 5615-90-7  | 1752839   | -              | Het   | pyrrole  | 1222      | 1.24       | 42         | 1162   | NA     | 975     | 904        |

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| Tentative Identification                  | CAS        | Peak Area | Health Effects | Class      | Subclass                  | t<sub>R</sub> (s) | 2t<sub>R</sub> (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse<sup>1</sup> | Similarity<sup>1</sup> |
|------------------------------------------|------------|-----------|----------------|------------|---------------------------|------------------|-----------------|------------|----------|----------|----------------------|------------------------|
| Pyrazine, 2-methyl-6-(1-propenyl)-, (E)- | 18217-81-7 | 76993     | -              | Het        | pyrazine                  | 1224             | 0.525           | 133        | 1163     | NA       | 882                  | 783                    |
| Benzene, (1-methylene-2-propenyl)-      | 13544-59-7 | 109190    | -              | HC         | monocyclic aromatic HC    | 1230             | 0.45            | 129        | 1166     | NA       | 894                  | 807                    |
| cis-p-mentha-1(7),8-dien-2-ol           | 2288-18-8  | 183072    | -              | Oxy        | alcohol                  | 1230             | 0.485           | 67         | 1166     | 1165     | 874                  | 868                    |
| Naphthalene, 1,2,3,4-tetrahydro-        | 122-46-3   | 121012    | -              | HC         | polycyclic aromatic HC    | 1232             | 0.42            | 104        | 1167     | 1166     | 878                  | 843                    |
| 2-Butanone, 4-(5-methyl-2-furanyl)-     | 13679-56-6 | 252019    | -              | Het        | furan                    | 1232             | 0.71            | 95         | 1167     | 1160     | 834                  | 773                    |
| m-Cresyl acetate                      | 119-64-2   | 197245    | X              | Oxy        | ester                    | 1232             | 0.775           | 108        | 1167     | NA       | 901                  | 827                    |
| Benzene, 1-methyl-4-butyl              | 1595-05-7  | 349972    | -              | HC         | polycyclic aromatic HC    | 1234             | 0.41            | 105        | 1168     | 1158     | 826                  | 843                    |
| Benzeneacetonitrile, á-methyl-         | 1823-91-2  | 120324    | -              | Nit        | nitrile                  | 1234             | 0.965           | 116        | 1169     | NA       | 930                  | 838                    |
| trans-p-mentha-1(7),8-dien-2-ol        | 2102-62-7  | 266318    | -              | Oxy        | alcohol                  | 1236             | 0.485           | 67         | 1169     | NA       | 856                  | 842                    |
| 1-Propanone, 1-phenyl-                 | 935-28-4   | 653705    | -              | Oxy        | ketone                   | 1236             | 0.71            | 105        | 1170     | 1173     | 924                  | 919                    |
| Egomaketone                             | 59204-74-9 | 579204    | X              | Oxy        | ketone                   | 1238             | 0.34            | 95         | 1170     | NA       | 798                  | 785                    |
| Cycloprop[a]indene, 1,1a,6,6a-tetrahydro- | 6909-19-9 | 241364    | -              | HC         | polycyclic aromatic HC    | 1240             | 0.455           | 130        | 1172     | NA       | 936                  | 915                    |
| Carane, 4,5-epoxy-, trans              | 20547-99-3 | 135133    | -              | Oxy        | epoxide                  | 1240             | 0.995           | 67         | 1172     | 1179     | 805                  | 769                    |
| 1,4-Cyclohexanedione, 2,2,6-trimethyl-  | 15677-15-3 | 83409     | -              | Oxy        | ketone                   | 1240             | 1.225           | 42         | 1172     | 1170     | 901                  | 764                    |
| Pyrrolidine, 1-acetyl-                 | 4030-18-6  | 157478    | -              | Het        | pyrrole                  | 1240             | 1.38            | 70         | 1172     | 1162     | 902                  | 808                    |
| 1H-Pyrrole-2,5-dione, 3,4-dimethyl-    | 17825-86-4 | 587037    | -              | Het        | pyrrole                  | 1242             | 1              | 125        | 1173     | NA       | 976                  | 827                    |
| 6-Ethyl-5,6-dihydro-2H-pyran-2-one     | 19895-35-3 | 3978068   | -              | Oxy        | ketone                   | 1244             | 1.44            | 68         | 1174     | NA       | 928                  | 919                    |
| Tentative Identification                                      | CAS      | Peak Area | Health Effects | Class | Subclass     | $1_{\text{R}}$ (s) | $2_{\text{R}}$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|--------------------------------------------------------------|----------|-----------|----------------|-------|--------------|---------------------|---------------------|------------|----------|----------|----------|------------|
| Phenol, 4-ethyl-                                             | 123-07-9 | 7046087   | X              | Oxy   | alcohol      | 1246                | 0.47                | 107        | 1175     | 1173     | 935      | 934        |
| Benzene, (1-ethylpropyl)-                                   | 1196-58-3| 165973    | -              | HC    | monocyclic   | 1250                | 0.385               | 119        | 1177     | NA       | 753      | 795        |
| Ethanal, 1-(4-methylphenyl)-                                | 122-00-9 | 779704    | X              | Oxy   | ketone       | 1250                | 0.795               | 119        | 1177     | 1177     | 971      | 938        |
| Benzonitrile, 3,5-dimethyl-                                 | 22445-42-7| 293860   | -              | Nit   | nitrile      | 1254                | 0.87                | 116        | 1179     | NA       | 914      | 928        |
| Phenol, 1-methyl-4-(1-methyl-2-propenyl)-                    | 1438-94-4| 276575    | -              | HC    | monocyclic   | 1258                | 0.395               | 131        | 1181     | 1190     | 871      | 875        |
| 1H-Pyrrole, 1-(2-furanyl)methyl-                            | 97664-18-1| 462250   | X              | Het   | pyrrole      | 1258                | 0.56                | 81         | 1181     | 1182     | 922      | 873        |
| Benzaldehyde, 2-methoxy-1,1-Dodecadiene                      | 89-74-7  | 208219    | -              | Nit   | amine        | 1260                | 0.78                | 108        | 1182     | 1181     | 867      | 771        |
| Phenol, 2,3-dimethyl-                                        | 526-75-0 | 806665    | -              | Oxy   | alcohol      | 1264                | 0.48                | 107        | 1184     | 1184     | 930      | 925        |
| Ethylidene cyclooctane                                      | 19780-51-9| 181577   | -              | HC    | alicyclic    | 1270                | 0.99                | 95         | 1188     | NA       | 737      | 765        |
| Phenol, 2-(1-methylethyl)-                                  | 88-60-8  | 454460    | X              | Oxy   | alcohol      | 1272                | 0.47                | 121        | 1189     | 1184     | 869      | 904        |
| 2-Methoxy-5-methylphenol                                    | 1195-09-1| 27551     | M              | Oxy   | ether        | 1274                | 0.615               | 138        | 1190     | 1191     | 880      | 775        |
| 2-Cyclohexen-1-one, 4-(1-methylethyl)-                      | 500-02-7 | 94193     | -              | Oxy   | ketone       | 1276                | 0.755               | 96         | 1191     | 1191     | 754      | 815        |
| Ethanone, 1-(3-methylphenyl)-                               | 585-74-0 | 914929    | -              | Oxy   | ketone       | 1276                | 0.8                 | 119        | 1191     | 1192     | 943      | 971        |
| 2,5-Dimethylbenzonitrile                                    | 13730-09-1| 527961   | X              | Nit   | nitrile      | 1276                | 0.895               | 116        | 1191     | NA       | 816      | 887        |
| 1-Dodecene                                                  | 5779-94-2| 673939    | -              | HC    | alkene       | 1278                | 0.3                  | 56         | 1192     | 1192     | 922      | 919        |
| (5Z)-5-DODECENE                                             | 112-41-4 | 87334     | -              | HC    | alkene       | 1278                | 0.305               | 81         | 1192     | 1184     | 921      | 922        |
| 1H-Indene, 2,3-dihydro-1,1-dimethyl-                         | 7206-19-1| 738489    | -              | HC    | polycyclic   | 1278                | 0.39                 | 131        | 1192     | NA       | 895      | 890        |
| 2-Decanone                                                  | 6909-20-2| 268380    | -              | Oxy   | ketone       | 1278                | 0.66                | 58         | 1192     | 1192     | 888      | 846        |
| Benzaldehyde, 2,5-dimethyl-                                  | 4912-92-9| 39704     | -              | Oxy   | aldehyde     | 1278                | 0.72                | 133        | 1192     | NA       | 895      | 785        |
| Tentative Identification                  | CAS     | Peak Area | Health Effects | Subclass       | $t_R$ (s) | $t_R'$ (s) | Quant | Mass   | Exp. RI | Lib. RI | Reverse | Similarity |
|------------------------------------------|---------|-----------|----------------|----------------|----------|-----------|-------|--------|---------|---------|---------|------------|
| Naphthalene                              | 91-20-3 | 4101274   | G2B            | HC             | 1280     | 0.55      | 128   | 1193   | 1192   | 952     | 956     |            |
| Phenol, 2-methoxy-4-methyl-              | 93-51-6 | 861658    | M              | Oxy alcohol    | 1280     | 0.64      | 123   | 1193   | 1193   | 940     | 938     |            |
| 2-Cyclohexen-1-one, 4-ethyl-4-methyl-    | 17429-32-2 | 292580    | -              | Oxy ketone     | 1282     | 0.99      | 95    | 1194   | NA     | 784     | 753     |            |
| 4-Dodecene, (E)-                        | 2030-84-4 | 61083     | -              | HC alkene      | 1284     | 0.29      | 56    | 1195   | NA     | 885     | 846     |            |
| 2-Piperidinone                           | 675-20-7 | 219287    | X              | Nit lactam     | 1284     | 1.385     | 99    | 1195   | NA     | 938     | 842     |            |
| Dodecane                                 | 112-40-3 | 1305887   | -              | HC alkane      | 1292     | 0.29      | 57    | 1199   | 1200   | 936     | 933     |            |
| (-)-alpha-Terpineol                      | 32780-06-6 | 70758     | -              | Oxy alcohol    | 1292     | 0.465     | 59    | 1199   | 1192   | 895     | 832     |            |
| (S)-(++)-2',3'-'Dideoxyribonolactone     | 10482-56-1 | 2880815   | X              | Oxy lactone    | 1292     | 1.505     | 85    | 1200   | NA     | 913     | 901     |            |
| Benzene, 1,4-diethyl-2-methyl-           | 13632-94-5 | 154210    | -              | HC monocyclic aromatic HC | 1294     | 0.38      | 133   | 1200   | NA     | 877     | 806     |            |
| 4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-  | 1073-96-7 | 146818    | -              | Het pyran      | 1294     | 0.64      | 142   | 1200   | 1205   | 857     | 752     |            |
| 1,5-Cyclohexadiene-1-carboxyalddehyde,  | 97997-08-5 | 61260     | -              | Oxy aldehyde   | 1300     | 0.69      | 91    | 1204   | NA     | 922     | 765     |            |
| 4,4-dimethyl-                            |          |           |                |                |          |           |      |        |        |         |         |            |
| Acetone peroxide                         | 1073-91-2 | 735872    | -              | Oxy peroxide   | 1300     | 1.81      | 43    | 1205   | NA     | 915     | 778     |            |
| 3-Dodecene, (Z)-                         | 7206-28-2 | 270367    | -              | HC alkene      | 1302     | 0.29      | 56    | 1205   | NA     | 877     | 871     |            |
| p-Ethylbenzonitrile                      | 25309-65-3 | 77236     | -              | Nit nitrile    | 1302     | 0.93      | 116   | 1205   | NA     | 915     | 805     |            |
| 2,3-Dimethylbenzonitrile                 | 5724-56-1 | 189138    | X              | Nit nitrile    | 1308     | 0.89      | 116   | 1209   | NA     | 841     | 879     |            |
| Phenol, 2,4,6-trimethyl-                 | 527-60-6  | 399622    | M              | Oxy alcohol    | 1310     | 0.47      | 121   | 1210   | 1211   | 964     | 915     |            |
| Benzene, 1-ethyl-4-(1-methyl)ethy-       | 4218-48-8 | 117499    | -              | HC monocyclic aromatic HC | 1312     | 0.38      | 133   | 1211   | NA     | 876     | 824     |            |
| Benzene, 1,2-diethyl-4,5-dimethyl-       | 52095-40-6 | 52769    | -              | HC monocyclic aromatic HC | 1314     | 0.365     | 119   | 1212   | NA     | 808     | 777     |            |
| Tentative Identification                                      | CAS     | Peak Area | Health Effects | Class          | Subclass      | \( t_R (s) \) | \( 2 t_R (s) \) | Quant Mass | Exp. RI† | Lib. RI‡ | Reverse† | Similarity‡ |
|--------------------------------------------------------------|---------|-----------|----------------|----------------|---------------|---------------|---------------|------------|---------|---------|---------|-----------|
| 1-(2-Vinylphenyl)ethanone                                     | 19961-07-0 | 384294    | -              | Oxy            | ketone        | 1314          | 0.485         | 131        | 1212    | NA      | 809     | 816      |
| Undecane, 2,6-dimethyl-                                       | 17301-23-4 | 1547981   | -              | HC             | alkane        | 1316          | 0.3          | 57         | 1213    | 1213    | 947     | 929      |
| Benzenamine, 2-(1-methylene)-                                 | 52562-19-3 | 73592     | -              | Nit            | amine         | 1316          | 0.62         | 117        | 1213    | NA      | 841     | 779      |
| 5,6,7,8-Tetrahydroquinoxaline                                 | 34413-35-9 | 52179     | -              | Nit            | aza-arene     | 1318          | 0.535        | 134        | 1214    | 1212    | 899     | 852      |
| Ethyl 4-pyridyl ketone                                        | 1701-69-5 | 74249     | X              | Het            | pyridine      | 1320          | 0.875        | 106        | 1215    | NA      | 865     | 760      |
| 2-Caren-10-ol                                                 | 6846-50-0 | 54218     | X              | Oxy            | alcohol       | 1324          | 0.77         | 107        | 1218    | NA      | 754     | 804      |
| Benzo furan, 4,7-dimethyl-                                    | 28715-26-6 | 124672    | -              | Het            | furan         | 1326          | 0.5          | 145        | 1219    | 1220    | 883     | 872      |
| 1-Nonanol, 4,8-dimethyl-                                      | 33933-80-1 | 217734    | -              | Oxy            | alcohol       | 1328          | 0.3          | 56         | 1220    | 1229    | 822     | 853      |
| Cyclohex anone, 2-(1-methylene)-                              | 13747-73-4 | 170885    | -              | Oxy            | ketone        | 1330          | 0.945        | 67         | 1221    | NA      | 806     | 785      |
| Cinnamaldehyde, \( \alpha \)-methyl-                         | 1196-67-4 | 827995    | X              | Oxy            | aldehyde      | 1332          | 0.495        | 145        | 1222    | NA      | 787     | 795      |
| 6-Dodecylene                                                  | 6975-99-1 | 206421    | -              | HC             | alkene        | 1338          | 0.325        | 54         | 1226    | NA      | 850     | 837      |
| Benzene, 2-ethenyl-1,3,5-trimethyl-                           | 769-25-5 | 251147    | -              | HC             | monocyclic    | 1338          | 0.405        | 131        | 1226    | 1224    | 914     | 900      |
| 4-Methyl-2H-chromene                                          | 21776-94-3 | 136967    | -              | Het            | pyran         | 1338          | 0.51         | 145        | 1226    | NA      | 764     | 838      |
| (Z)-3-Phenylacrylaldehyde                                     | 57194-69-1 | 31949     | -              | Oxy            | aldehyde      | 1340          | 0.82         | 131        | 1227    | 1223    | 754     | 843      |
| Phenol, 2-propyl-                                             | 1007-32-5 | 385352    | -              | Oxy            | alcohol       | 1342          | 0.435        | 107        | 1228    | 1229    | 755     | 778      |
| 1-Phenyl-2-butanone                                           | 20548-00-9 | 224688    | -              | Oxy            | ketone        | 1342          | 0.74         | 57         | 1228    | NA      | 888     | 795      |
| 4-Methyleneisophorone                                         | 644-35-9 | 69978     | X              | Oxy            | ketone        | 1342          | 0.945        | 107        | 1228    | 1224    | 860     | 804      |
| 3-Phenylfuran-                                                | 13679-41-9 | 147003    | -              | Het            | furan         | 1344          | 0.53         | 115        | 1229    | 1228    | 917     | 800      |
| 2,3-Dihydro-benzofuran                                        | 496-16-2 | 3841449   | -              | Het            | furan         | 1348          | 0.48         | 120        | 1231    | 1226    | 911     | 903      |
| Phenol, 3-(1-methylene)-                                      | 618-45-1 | 970578    | X              | Oxy            | alcohol       | 1352          | 0.435        | 121        | 1234    | 1229    | 830     | 899      |
| 2,5-Dimethylbenzoxazole                                       | 17583-40-3 | 57595     | -              | Nit            | oxazole       | 1354          | 0.535        | 147        | 1235    | NA      | 890     | 844      |
| Benzonitrile, 2-(methylamino)-                                | 5676-58-4 | 411641    | X              | Nit            | nitrile       | 1354          | 0.59         | 131        | 1235    | NA      | 888     | 880      |
| Phenol, 4-ethyl-3-methyl-                                     | 1123-94-0 | 423310    | -              | Oxy            | alcohol       | 1360          | 0.43         | 121        | 1238    | 1239    | 832     | 889      |
Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification | CAS     | Peak Area | Health Effects | Class      | Subclass       | \( t_R \) (s) | Health Effects | Class      | Subclass       | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|--------------------------|---------|-----------|----------------|------------|----------------|---------------|----------------|------------|----------------|------------|---------|---------|---------|------------|
| Isoquinoline, 3,4-dihydro- | 3230-65-7 | 550157    |                | Nit        | aza-arene      | 1360          | 0.645          | 130        | 1238           | NA         | 834    | 821     |         |            |
| Phenol, 2,3,6-trimethyl- | 20189-42-8 | 115369    |                | Oxy        | alcohol        | 1362          | 0.475          | 120        | 1239           | 1239       | 885    | 833     |         |            |
| 1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl- | 2416-94-6 | 468503    | X              | Het        | pyrrole        | 1362          | 0.94           | 139        | 1240           | 1239       | 925    | 907     |         |            |
| Benzene, 3-hexenyl-      | 35008-86-7 | 231660    |                | HC         | monocyclic aromatic HC | 1364          | 0.385          | 91         | 1241           | NA         | 860    | 760     |         |            |
| Benzene, 1-methoxy-2-(1-methylethenyl)- | 10278-02-1 | 53397     |                | Oxy        | ether          | 1368          | 0.685          | 133        | 1243           | NA         | 780    | 822     |         |            |
| Benzenepropanenitrile   | 645-59-0  | 2605873   |                | Nit        | nitrile        | 1368          | 1.01           | 91         | 1243           | 1243       | 944    | 936     |         |            |
| Diacetin                | 25395-31-7 | 2874087   | X              | Oxy        | ester          | 1370          | 1.065          | 43         | 1244           | NA         | 957    | 952     |         |            |
| Benzene, [(2,2-dimethylcyclopropyl)methyl]- | 36939-18-1 | 783620    |                | HC         | monocyclic aromatic HC | 1372          | 0.375          | 69         | 1245           | NA         | 825    | 820     |         |            |
| 2-Butanone, 4-phenyl-    | 2550-26-7 | 179662    |                | Oxy        | ketone         | 1374          | 0.79           | 105        | 1246           | 1251       | 892    | 881     |         |            |
| Isoquinoline             | 119-65-3  | 771054    | M              | Nit        | aza-arene      | 1378          | 0.63           | 129        | 1249           | 1255       | 950    | 942     |         |            |
| Phenol, 3-ethyl-5-methyl- | 698-71-5  | 311869    |                | Oxy        | alcohol        | 1380          | 0.445          | 121        | 1250           | NA         | 870    | 900     |         |            |
| 2-Hexanoylfuran          | 14360-50-0 | 134937    |                | Het        | furan          | 1380          | 0.79           | 110        | 1250           | 1239       | 839    | 762     |         |            |
| 2-Ethyl-1-H-indene       | 17059-50-6 | 292758    |                | HC         | polycyclic aromatic HC | 1382          | 0.44           | 129        | 1251           | NA         | 861    | 784     |         |            |
| Benzene, 1-methyl-3-(1-methyl-2-propenyl)- | 52161-57-6 | 208093    |                | HC         | monocyclic aromatic HC | 1390          | 0.385          | 131        | 1255           | NA         | 847    | 841     |         |            |
| Ethanone, 1-(2,4-dimethylphenyl)-(3E)-3-Nonen-1-ol | 89-72-5  | 49494     | X              | Oxy        | ketone         | 1390          | 0.67           | 133        | 1256           | NA         | 893    | 810     |         |            |
| (3E)-3-Nonen-1-ol        | 10339-61-4 | 76837     |                | Oxy        | alcohol        | 1392          | 0.315          | 68         | 1257           | NA         | 842    | 808     |         |            |
| 1H-Indene, 1,1-dimethyl- | 32267-71-3 | 380513    |                | HC         | polycyclic aromatic HC | 1392          | 0.445          | 129        | 1257           | NA         | 858    | 808     |         |            |

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Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification                                                                 | CAS       | Peak Area | Health Effects | Class   | Subclass             | 1tR (s) | 2tR (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|------------------------------------------------------------------------------------------|-----------|-----------|----------------|---------|----------------------|---------|---------|------------|----------|----------|----------|--------------|
| 2(3H)-Benzofuranone, 3-methyl-                                                          | 18636-55-0| 36565     | -              | Oxy     | ketone               | 1392    | 0.875   | 120        | 1257     | NA       | 935      | 755         |
| (2E,4Z)-2,4-Dodecadiene                                                                | 939-23-1  | 195690    | -              | HC      | alkene               | 1400    | 0.32    | 68         | 1261     | NA       | 814      | 799         |
| Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-                                         | 74663-83-5| 39403     | -              | HC      | polycyclic aromatic  | 1400    | 0.35    | 159        | 1261     | 1264     | 764      | 786         |
| 4-Ethylphenyl acetate                                                                   | 3245-23-6 | 126587    | -              | Oxy     | ester                | 1400    | 0.73    | 107        | 1261     | NA       | 869      | 798         |
| Benzene, (1-methylpentyl)-                                                              | 03/01/6031| 273787    | -              | HC      | monocyclic aromatic  | 1402    | 0.365   | 105        | 1262     | NA       | 854      | 811         |
| Naphthalene, 1,2-dihydro-2-methyl-                                                      | 21564-79-4| 1513265   | -              | HC      | polycyclic aromatic  | 1402    | 0.44    | 129        | 1262     | NA       | 888      | 896         |
| Benzene, hexyl-                                                                         | 1077-16-3 | 324906    | -              | HC      | monocyclic aromatic  | 1404    | 0.37    | 92         | 1263     | 1263     | 884      | 878         |
| Dodecane, 2-methyl-                                                                     | 1560-97-0 | 88630     | -              | HC      | alkane               | 1406    | 0.29    | 57         | 1265     | 1265     | 896      | 827         |
| Phenol, 4-propyl-                                                                        | 645-56-7  | 913975    | -              | Oxy     | alcohol              | 1410    | 0.45    | 107        | 1267     | 1262     | 896      | 851         |
| Ethanone, 1-(2,5-dimethylphenyl)-                                                       | 2142-73-6 | 153409    | -              | Oxy     | ketone               | 1410    | 0.735   | 133        | 1267     | NA       | 820      | 863         |
| 2-Acetoxy-3-methyl-2-cyclopenten-1-one                                                  | 1196-22-1 | 92929     | -              | Oxy     | ketone               | 1414    | 1.365   | 112        | 1270     | NA       | 943      | 890         |
| Benzeneacetaldehyde                                                                     | 122-78-1  | 77589     | X              | Oxy     | aldehyde             | 1416    | 0.98    | 51         | 1271     | NA       | 906      | 851         |
| 2-Propyl-4-methylphenol                                                                  | 91-22-5   | 103039    | G2B            | Oxy     | alcohol              | 1420    | 0.455   | 121        | 1273     | NA       | 764      | 853         |
| Quinoline                                                                               | 4074-46-8 | 311612    | -              | Nit     | aza-arene            | 1420    | 0.7     | 129        | 1273     | 1255     | 946      | 900         |
| 1-Propanone, 1-(2-methylphenyl)-                                                        | 603-76-9  | 309360    | -              | Oxy     | ketone               | 1424    | 0.685   | 119        | 1275     | NA       | 928      | 881         |
| 1H-Indole, 1-methyl-                                                                     | 2040-14-4 | 152948    | -              | Nit     | aza-arene            | 1424    | 0.71    | 131        | 1275     | 1277     | 908      | 879         |
| 1H-Indene, 2,3-dimethyl-                                                                 | 4773-82-4 | 1149600   | -              | HC      | polycyclic aromatic  | 1426    | 0.48    | 129        | 1276     | NA       | 909      | 903         |

Continued on next page
| Tentative Identification | CAS      | Peak Area | Health Effects | Class Subclass | 1\(t_R\) (s) | 2\(t_R\) (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|--------------------------|----------|-----------|----------------|----------------|--------------|-------------|------------|---------|---------|----------|------------|
| Benzene, 1-cyclopenten-1-yl- | 824-22-6 | 145416    | -              | HC polycyclic aromatic HC | 1430        | 0.425       | 143        | 1278    | NA      | 857      | 780        |
| Benzene, 1,4-dimethyl-2-(2-methylpropyl)- | 2785-89-9 | 54389     | -              | HC monocyclic aromatic HC | 1432        | 0.365       | 119        | 1280    | NA      | 845      | 753        |
| Phenol, 4-ethyl-2-methoxy-3,4-Dimethyl-3-pyrrolin-2-one | 55669-88-0 | 768057    | -              | Oxy alcohol      | 1432        | 0.6         | 137        | 1280    | 1280    | 939      | 923        |
| Ethanone, 1-(2,5-dihydroxyphenyl)- | 490-78-8 | 368949    | X              | Oxy ketone      | 1440        | 0.695       | 137        | 1284    | NA      | 907      | 853        |
| Benzonitrile, 4-(1-methylethyl)- | 13816-33-6 | 79513     | X              | Nit nitrile     | 1440        | 0.845       | 130        | 1284    | NA      | 845      | 783        |
| Phenol, 2-ethyl-5-methyl-1H-Pyrrole, 1-phenyl-4-Hydroxy-2-methylacetophenone | 875-59-2 | 247139    | -              | Oxy alcohol      | 1442        | 0.48        | 121        | 1285    | NA      | 823      | 878        |
| 1H-Indene, 1-ethylidene- | 2471-83-2 | 101239    | -              | HC polycyclic aromatic HC | 1448        | 0.535       | 141        | 1289    | NA      | 821      | 932        |
| 1H-Indene, 2,3-dihydro-4,7-dimethyl- | 83-33-0   | 124652    | -              | HC polycyclic aromatic HC | 1446        | 0.395       | 131        | 1288    | 1282    | 830      | 815        |
| 1H-Inden-1-one, 2,3-dihydro-6682-71-9 | 6682-71-9 | 1611858   | -              | Oxy ketone      | 1446        | 0.84        | 104        | 1288    | 1285    | 968      | 955        |
| 1H-Indene, 1-ethylidene-2471-83-2 | 2471-83-2 | 101239    | -              | HC polycyclic aromatic HC | 1448        | 0.535       | 141        | 1289    | NA      | 821      | 932        |
| Ethanone, 1-(4-ethylphenyl)-2-Tridecene, (E)- | 93-55-0     | 77673     | X              | Oxy ketone      | 1448        | 0.73        | 133        | 1289    | 1295    | 888      | 809        |
| Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene-2443-46-1 | 2443-46-1 | 114850    | -              | HC polycyclic aromatic HC | 1454        | 0.495       | 141        | 1292    | NA      | 778      | 857        |
| 2-Undecanone | 112-12-9     | 189842    | X              | Oxy ketone      | 1454        | 0.625       | 58         | 1292    | 1292    | 899      | 820        |
| Hydroquinone | 123-31-9     | 1538373   | G3             | Oxy quinone      | 1460        | 0.545       | 110        | 1296    | NA      | 915      | 885        |
| Tentative Identification | CAS        | Peak Area | Health Effects | Class  | Subclass | $1_{IR}$ (s) | $2_{IR}$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|--------------------------|------------|-----------|----------------|--------|----------|--------------|--------------|------------|--------|--------|---------|-----------|
| 2-Tridecene, (Z)-        | 41446-59-7 | 26349     | -              | HC     | alkene   | 1462         | 0.295        | 57         | 1297   | 1302   | 893     | 817       |
| Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl- | 2219-78-5 | 123665    | -              | HC     | polycyclic aromatic HC | 1464 | 0.37 | 145     | 1298   | 1318   | 851     | 831       |
| Naphthalene, 1,2,3,4-tetrahydro-5-methyl- | 25419-33-4 | 44384     | -              | HC     | polycyclic aromatic HC | 1464 | 0.415 | 118     | 1298   | 1279   | 854     | 803       |
| 2-Ethyl-4,5-dimethylphenol | 2809-64-5 | 311257    | -              | Oxy    | alcohol  | 1464         | 0.43         | 135        | 1298   | 1300   | 909     | 835       |
| Tridecane                | 629-50-5   | 2696030   | -              | HC     | alkane   | 1466         | 0.29         | 57         | 1299   | 1300   | 963     | 951       |
| Indole                   | 120-72-9   | 4495705   | -              | Nit    | arene    | 1470         | 0.64         | 117        | 1302   | 1303   | 937     | 936       |
| 2-Allylphenol            | 4360-47-8  | 212451    | -              | Oxy    | alcohol  | 1472         | 0.48         | 134        | 1303   | NA     | 836     | 800       |
| Cinnamonitrile           | 1745-81-9  | 533463    | X              | Nit    | nitrile  | 1472         | 0.96         | 129        | 1303   | 1301   | 925     | 908       |
| 3-Tridecene, (E)-        | 41446-57-5 | 314144    | -              | HC     | alkene   | 1474         | 0.29         | 69         | 1304   | NA     | 921     | 904       |
| Naphthalene, 2-methyl-   | 91-57-6    | 2312506   | -              | HC     | polycyclic aromatic HC | 1476 | 0.54 | 142     | 1305   | 1305   | 956     | 930       |
| 1-Ethyl-1,2,3,4-tetrahydroanaphthalene | 13556-58-6 | 100871    | -              | HC     | polycyclic aromatic HC | 1480 | 0.405 | 131     | 1308   | 1309   | 861     | 797       |
| Ethanone, 1-(2-hydroxy-5-methylphenyl)- | 1450-72-2 | 127899    | -              | Oxy    | ketone   | 1482         | 0.85         | 135        | 1309   | 1316   | 760     | 836       |
| Quinoxaline, 2-methyl-    | 7239-23-8  | 121072    | -              | Nit    | arene    | 1484         | 0.54         | 144        | 1310   | 1304   | 909     | 875       |
| 3-Butyl-2-hydroxyl-2-cyclopenten-1-one | 17496-14-9 | 63789     | -              | Oxy    | ketone   | 1490         | 0.67         | 112        | 1314   | NA     | 838     | 769       |
| 1H-Inden-1-one, 2,3-dihydro-2-methyl- | 29798-72-9 | 618867    | -              | Oxy    | ketone   | 1490         | 0.75         | 131        | 1314   | NA     | 915     | 913       |
| 2-Methyl-6-propylphenol  | 3520-52-3  | 188644    | -              | Oxy    | alcohol  | 1492         | 0.42         | 121        | 1315   | 1320   | 856     | 791       |
| 2,5-Diethylphenol        | 876-20-0   | 293612    | -              | Oxy    | alcohol  | 1494         | 0.42         | 135        | 1316   | NA     | 897     | 837       |
| 1H-Inden-1-one, 2,3-dihydro-3,3-dimethyl- | 91-63-4   | 380673    | M              | Oxy    | ketone   | 1496         | 0.465        | 145        | 1318   | NA     | 774     | 766       |
| Quinoline, 2-methyl-      | 77822-47-0 | 254318    | -              | Nit    | arene    | 1496         | 0.555        | 143        | 1318   | 1313   | 945     | 914       |
Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification | CAS        | Peak Area | Health Effects | Class       | Subclass                  | 1R (s) | 2R (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|-------------------------|------------|-----------|----------------|-------------|---------------------------|--------|--------|------------|--------|--------|---------|------------|
| 2-Methoxy-4-vinylphenol | 26465-81-6 | 2531743   | -              | Oxy ether   |                           | 1496   | 0.62   | 135        | 1318   | 1317   | 943     | 938        |
| 2-Ethylhexyl butyrate   | 25415-84-3 | 331407    | -              | Oxy ester   |                           | 1500   | 0.48   | 71         | 1320   | 1321   | 897     | 867        |
| Triasteronone           | 1903-34-0  | 352892    | -              | Oxy ketone  | monocyclic aromatic HC    | 1500   | 0.82   | 91         | 1320   | NA     | 800     | 820        |
| 1-Buten-3-ynylbenzene   | 146276-26-8| 100531    | -              | HC          |                           | 1502   | 0.555  | 128        | 1321   | NA     | 950     | 807        |
| Naphthalene, 1-methyl   | 90-12-0    | 1937024   | -              | HC          | polycyclic aromatic HC    | 1504   | 0.53   | 142        | 1323   | 1315   | 936     | 941        |
| 1-Cyclohexyl-1-pentyne  | NA         | 213071    | -              | HC          | alicyclic HC               | 1506   | 0.32   | 93         | 1324   | NA     | 754     | 824        |
| Trinoranastreptene      | 35587-60-1 | 38109     | -              | HC          | polycyclic aromatic HC    | 1508   | 0.4    | 145        | 1325   | NA     | 922     | 753        |
| 1-Methylindan-2-one     | 86160-98-7 | 390441    | -              | Oxy ketone  |                           | 1508   | 0.84   | 131        | 1325   | NA     | 906     | 901        |
| Quinoline, 5-methyl     | 7661-55-4  | 216317    | M              | Nit aza-arene|                           | 1510   | 0.52   | 143        | 1326   | NA     | 921     | 886        |
| Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl- | 527-54-8  | 48500     | -              | HC          | polycyclic aromatic HC    | 1512   | 0.395  | 118        | 1327   | NA     | 852     | 764        |
| Phenol, 3,4,5-trimethyl- | 4175-54-6  | 132606    | -              | Oxy alcohol |                           | 1512   | 0.505  | 121        | 1328   | 1331   | 854     | 887        |
| 2,3,5,6-Tetramethylbenzo-1,4-quinone | 527-17-3 | 140508 | M              | Oxy quinone |                           | 1514   | 0.72   | 121        | 1329   | 1326   | 910     | 844        |
| 1H-Inden-5-ol, 2,3-dihydro- | 1470-94-6 | 114802    | X              | Oxy alcohol | monocyclic aromatic HC    | 1516   | 0.485  | 133        | 1330   | 1335   | 873     | 819        |
| 1-Isoprenyl-2-isopropylbenzene | 24524-55-8 | 163351    | -              | HC          | monocyclic aromatic HC    | 1520   | 0.39   | 145        | 1332   | NA     | 867     | 822        |
| Benzene, [(1-methylethylidene)cyclopropyl]-, (R)- | 5557-93-7 | 155928    | -              | HC          | monocyclic aromatic HC    | 1520   | 0.42   | 143        | 1332   | NA     | 771     | 884        |
| Phenol, 2-(1-methylpropyl)- | 88-69-7  | 227832    | -              | Oxy alcohol |                           | 1522   | 0.425  | 121        | 1334   | NA     | 770     | 811        |

Continued on next page
| Tentative Identification                                      | CAS          | Peak Area | Health Effects | Class | Subclass       | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse† | Similarity‡ |
|--------------------------------------------------------------|--------------|-----------|----------------|-------|----------------|----------|-----------|------------|--------|--------|----------|-------------|
| 2-Methyl-7-exo-vinylbicyclo[4.2.0]oct-1(2)-ene               | 107914-89-6  | 48110     | -              | HC    | polycyclic     | 1522     | 0.735     | 105        | 1334   | NA     | 843      | 752         |
| Benzopyrimidine, 3,4-dihydro-                                | 1904-64-9    | 88191     | -              | Het   | pyrimidine     | 1522     | 0.76      | 131        | 1334   | NA     | 908      | 770         |
| 1-(3-Methylphenyl)4-methyl-3-pentene                         | 51082-26-9   | 312150    | -              | HC    | monocyclic     | 1524     | 0.36      | 105        | 1335   | NA     | 871      | 851         |
| (3E)-3-Methyl-4-phenyl-3-butene-2-one                        | 1901-26-4    | 339783    | X              | Oxy   | ketone         | 1526     | 0.49      | 145        | 1336   | NA     | 818      | 806         |
| Phosphonic acid, ethyl-, diethyl ester                       | 78-38-6      | 86736     | X              | Misc  | phosphonate    | 1526     | 1.185     | 54         | 1337   | NA     | 999      | 901         |
| 1H-Inden-1-one, 2,3,4,5,6,7-hexahydro-                       | 22118-00-9   | 52609     | -              | Oxy   | ketone         | 1528     | 0.925     | 136        | 1338   | NA     | 916      | 830         |
| Pyrrole[1,2-alpyrazine, 3-methyl-                            | 102-76-1     | 294069    | -              | Het   | pyrazine       | 1530     | 0.765     | 132        | 1339   | NA     | 906      | 864         |
| Triacetin                                                    | 64608-61-3   | 33719502  | -              | Oxy   | ester          | 1530     | 1.17      | 103        | 1339   | 1339   | 938      | 935         |
| Isoquinoline, 3-methyl-                                      | 1125-80-0    | 93343     | M              | Nit   | aza-arene      | 1534     | 0.57      | 143        | 1341   | NA     | 750      | 815         |
| 1-Methyl-4-(1-pentyn-1-yl)benzene                            | NA           | 192889    | M              | HC    | monocyclic     | 1542     | 0.43      | 129        | 1346   | NA     | 816      | 845         |
| Benzylidenemalonaldehyde                                     | 825-54-7     | 165838    | -              | Oxy   | aldehyde       | 1542     | 0.52      | 132        | 1346   | NA     | 856      | 874         |
| 1-Naphthalenol, 4-methyl-                                    | 10240-08-1   | 69143     | -              | Oxy   | alcohol        | 1544     | 0.505     | 157        | 1347   | NA     | 841      | 817         |
| 11-Tridecyn-1-ol                                            | 33925-75-6   | 76306     | -              | Oxy   | alcohol        | 1546     | 0.305     | 68         | 1348   | NA     | 847      | 776         |
| Benzoaldehyde, ethyl-                                       | 53951-50-1   | 99699     | -              | Oxy   | aldehyde       | 1552     | 0.495     | 134        | 1352   | NA     | 807      | 837         |
| Phenol, 2,6-dimethoxy-                                      | 91-10-1      | 851551    | -              | Oxy   | ether          | 1552     | 0.71      | 154        | 1352   | 1353   | 928      | 926         |
| Nicotine                                                    | 54-11-5      | 26793591  | M              | Het   | pyridine       | 1560     | 0.575     | 133        | 1357   | 1360   | 948      | 948         |
| Naphthalene, 1,2,3,4-tetrahydro-1-propyl-                    | 25586-57-6   | 192730    | -              | HC    | polycyclic     | 1562     | 0.375     | 131        | 1358   | NA     | 859      | 828         |

Continued on next page
| Tentative Identification                          | CAS      | Peak Area | Health Effects | Class    | Subclass                              | $t_R$ (s) | $t_R$ (s) | Quant Mass | Exp. RI$^\ast$ | Lib. RI$^\ast$ | Reverse$^1$ | Similarity$^1$ |
|------------------------------------------------|----------|-----------|----------------|----------|---------------------------------------|----------|-----------|------------|---------------|----------------|-------------|---------------|
| Benzene, 2-heptenyl-, (Z)-                     | 54725-18-7 | 59911     | -              | HC       | monocyclic aromatic HC                | 1562     | 0.385     | 104        | 1358          | NA             | 805         | 754           |
| Phenol, 2-methoxy-3-(2-propenyl)-              | 66324-83-2 | 101576    | -              | Oxy ether| polycyclic aromatic HC               | 1562     | 0.565     | 164        | 1358          | 1362           | 861         | 859           |
| 7-Methylindan-1-one                            | 39627-61-7 | 330314    | -              | Oxy ketone| polycyclic aromatic HC              | 1564     | 0.68      | 146        | 1360          | NA             | 880         | 894           |
| Solanone                                       | 54868-48-3 | 4316592   | -              | Oxy ketone| polycyclic aromatic HC              | 1566     | 0.64      | 93         | 1361          | NA             | 934         | 919           |
| Naphthalene, 1,2-dihydro-1,1,6-trimethyl-      | 87791-00-2 | 328122    | -              | HC       | polycyclic aromatic HC               | 1570     | 0.39      | 142        | 1363          | 1364           | 906         | 885           |
| Phenol, 2-(1,1-dimethyl-ethyl)-5-methyl-       | 30364-38-6 | 68974     | -              | Oxy alcohol| polycyclic aromatic HC         | 1570     | 0.4       | 149        | 1363          | 1365           | 908         | 773           |
| Tridecane, 2-methyl-                           | 6968-35-0  | 172858    | -              | HC       | monocyclic aromatic HC               | 1572     | 0.29      | 57         | 1364          | 1364           | 899         | 854           |
| Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-| 1007-91-6  | 365322    | -              | HC       | polycyclic aromatic HC               | 1572     | 0.38      | 159        | 1364          | NA             | 924         | 905           |
| Benzene, (1,1-dimethyl-2-butynyl)-             | 1560-96-9  | 284177    | -              | HC       | monocyclic aromatic HC               | 1572     | 0.42      | 143        | 1365          | NA             | 803         | 837           |
| 7-Hydroxy-1-indanone                           | 475-03-6   | 101062    | -              | Oxy ketone| monocyclic aromatic HC              | 1572     | 0.74      | 148        | 1365          | NA             | 855         | 825           |
| Quinoline, 8-methyl-                           | 611-32-5   | 221459    | M              | Nit aza-arene| monocyclic aromatic HC       | 1574     | 0.625     | 143        | 1366          | NA             | 935         | 907           |
| Benzene, 1,3-hexadienyl-                       | 1667-01-2  | 152436    | -              | HC       | monocyclic aromatic HC               | 1576     | 0.46      | 143        | 1367          | NA             | 787         | 815           |
| Ethanone, 1-(2,4,6-trimethylphenyl)-           | 41635-77-2 | 47589     | -              | Oxy ketone| monocyclic aromatic HC              | 1576     | 0.695     | 147        | 1367          | NA             | 875         | 753           |
| Benzene, heptyl-                               | 1078-71-3  | 289211    | -              | HC       | monocyclic aromatic HC               | 1578     | 0.37      | 92         | 1368          | 1368           | 858         | 815           |
| Phenol, 2-methoxy-4-propyl-                    | 2785-87-7  | 143665    | X              | Oxy ether| monocyclic aromatic HC              | 1578     | 0.58      | 137        | 1369          | 1369           | 838         | 790           |

Continued on next page
| Tentative Identification | CAS   | Peak Area | Health Effects | Class | Subclass     | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|-------------------------|-------|-----------|----------------|-------|--------------|-----------|-----------|------------|---------|---------|---------|------------|
| Tridecane, 3-methyl-    | 6418-41-3 | 134896   | -              | HC    | alkane       | 1582      | 0.29      | 57         | 1371   | 1371   | 796     | 762        |
| 1H-Indene, 1,1,3-trimethyl- | 2177-45-9 | 353320   | -              | HC    | polycyclic   | 1582      | 0.425     | 143        | 1371   | NA     | 829     | 835        |
| Phenol, 2-(2-methyl-2-propanyl)- | 612-58-8 | 55531    | M              | Oxy   | alcohol      | 1584      | 0.48      | 148        | 1372   | NA     | 834     | 789        |
| Quinoline, 3-methyl-    | 20944-88-1 | 105272   | -              | Nit   | aza-arene    | 1584      | 0.645     | 143        | 1372   | 1361   | 870     | 780        |
| 1H-Indole, 2-methyl-    | 95-20-5    | 175282   | X              | Nit   | aza-arene    | 1586      | 0.67      | 130        | 1373   | 1373   | 917     | 844        |
| 1,3-Dimethyl -1H-indole | 875-30-9   | 206229   | -              | Nit   | aza-arene    | 1588      | 0.62      | 144        | 1375   | 1383   | 906     | 883        |
| Farnesane               | 3891-98-3  | 1164068  | -              | HC    | sesquiterpene| 1590      | 0.3       | 71         | 1376   | 1376   | 938     | 929        |
| 2,3,5,6- Tétraméthylacétophénone | 2142-79-2 | 271421   | -              | Oxy   | ketone       | 1592      | 0.62      | 161        | 1377   | NA     | 836     | 827        |
| (E)-1-(2,3,6-trimethylphenyl)buta-1,3-diene (TPB, 1) | 18190-44-8 | 96034    | -              | HC    | monocyclic   | 1598      | 0.395     | 157        | 1381   | NA     | 820     | 757        |
| Ethanone, 1-[4-(1-methylethenyl)phenyl]- | 5359-046  | 289429   | -              | Oxy   | ketone       | 1598      | 0.605     | 145        | 1381   | NA     | 782     | 790        |
| N-[2-Hydroxyethyl]succinimide | NA      | 79013    | -              | Nit   | imide        | 1598      | 1.025     | 100        | 1381   | NA     | 864     | 783        |
| beta-Elemene            | 33880-83-0 | 39138    | -              | HC    | sesquiterpene| 1600      | 0.345     | 147        | 1382   | 1384   | 806     | 783        |
| (1-Methylpenta-1,3-dienyl)benzene | 116669-49-9 | 1333540  | -              | HC    | monocyclic   | 1602      | 0.45      | 143        | 1383   | NA     | 870     | 875        |
| Quinoline, 2,7-dimethyl-beta-Damascenone | 49826-53-1 | 94047    | -              | Nit   | aza-arene    | 1606      | 0.47      | 157        | 1386   | 1392   | 772     | 829        |
| beta-Damascenone        | 93-37-8    | 357561   | -              | Oxy   | ketone       | 1606      | 0.625     | 69         | 1386   | 1385   | 804     | 771        |
| 1(2H)-Naphthalenone, 3,4-dihydro- | 23726-93-4 | 61730    | -              | Oxy   | ketone       | 1606      | 0.78      | 118        | 1386   | NA     | 870     | 801        |
| Bicyclo[3.2.1]oct-2-ene, 3-methyl-4-methylene- | 529-34-0   | 212853   | -              | HC    | alicyclic    | 1606      | 1.055     | 91         | 1386   | NA     | 820     | 764        |
| Tentative Identification | CAS       | Peak Area | Health Effects | Class       | Subclass       | \( t_R \) (s) | 2\( t_R \) (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|-------------------------|-----------|-----------|----------------|-------------|----------------|--------------|--------------|------------|----------|----------|----------|------------|
| Benzene, (1,2,3-trimethyl-2-cyclopropen-1-yl)- | 6393-13-1 | 318725    | -              | HC          | monocyclic aromatic HC | 1610 | 0.46 | 143 | 1388 | NA | 849 | 874 |
| Methyl 5-oxo-2-pyrrolidinecarboxylate | 54571-66-3 | 704779    | -              | Het         | pyrrole        | 1610 | 1.495 | 84 | 1389 | 1391 | 912 | 826 |
| Biphenyl                | 92-52-4   | 647857    | G2A            | HC          | polycyclic aromatic HC | 1612 | 0.47 | 154 | 1389 | 1391 | 955 | 944 |
| 1H-Pyrrole, 1-(4-methylphenyl)- | 491-35-0 | 26567     | M              | Het         | pyrrole        | 1614 | 0.51 | 157 | 1390 | NA | 847 | 755 |
| Quinoline, 4-methyl-1-Tetracene | 82700-43-4 | 187270    | -              | Nit         | aza-arene      | 1614 | 0.65 | 143 | 1391 | 1391 | 943 | 884 |
| 3-Dodecen-1-ol          | 1120-36-1 | 1246422   | -              | HC          | alkene         | 1616 | 0.29 | 69 | 1392 | 1392 | 951 | 943 |
| 1H-Indole, 3-methyl-Pyrrol[1,2-a]pyrazine, 1,4-dimethyl- | 1626-86-5 | 60767     | -              | Nit         | aza-arene      | 1622 | 0.6 | 130 | 1395 | 1395 | 944 | 944 |
| 1H-Indene, 2,3-dihydro-1,1,3-trimethyl- | 2613-76-5 | 110883    | -              | HC          | polycyclic aromatic HC | 1628 | 0.375 | 145 | 1399 | NA | 908 | 857 |
| Tetradecane             | 629-59-4  | 2645724   | -              | HC          | alkene         | 1630 | 0.28 | 57 | 1400 | 1400 | 958 | 954 |
| 1H-Indene, 3-ethenyl-2,3-dihydro-1,1-dimethyl- | 612-60-2 | 118898    | M              | HC          | polycyclic aromatic HC | 1634 | 0.415 | 142 | 1403 | NA | 823 | 799 |
| 5-methyl-1H-Indole      | 614-96-0  | 571301    | -              | Nit         | aza-arene      | 1634 | 0.62 | 130 | 1403 | 1398 | 863 | 884 |
| Quinoline, 7-methyl-1H-Indole | 53909-98-1 | 94552     | -              | Nit         | aza-arene      | 1634 | 0.68 | 143 | 1403 | 1355 | 861 | 788 |
| 3-Tetracene, (Z)-       | 41446-67-7 | 148206    | -              | HC          | alkene         | 1636 | 0.28 | 56 | 1404 | 1385 | 928 | 922 |
| 2-Methylbiphenyl        | 54484-71-8 | 48017     | -              | HC          | polycyclic aromatic HC | 1638 | 0.4 | 168 | 1406 | 1404 | 876 | 815 |
| 3,4,6-trimethyl-1-Indanone | 1127-76-0 | 226119    | -              | Oxy         | ketone         | 1638 | 0.425 | 159 | 1406 | NA | 779 | 759 |

Continued on next page
| Tentative Identification                  | CAS   | Peak Area | Health Effects | Class     | Subclass     | $t_{R1}$ (s) | $t_{R2}$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|------------------------------------------|-------|-----------|----------------|-----------|-------------|--------------|--------------|------------|--------|--------|---------|----------|
| 1-Ethynaphthalene                        | 643-58-3 | 1106695 | X              | HC        | polycyclic aromatic HC | 1638 0.5 | 141 1406 | 1406 936 | 932    |        |         |
| 1-Phenylpyrrolidine                      | 4096-21-3 | 70981   | -              | Het       | pyrrole     | 1640 0.525 | 146 1407 | NA 815   | 893    |        |         |
| trans-beta-Caryophyllene                 | 621-59-0 | 598182  | M              | HC        | sesquiterpene | 1642 0.33 | 93 1408 | 1406 844 | 804    |        |         |
| Isovanillin                              | 87-44-5  | 243745   | -              | Oxy       | aldehyde    | 1642 0.895 | 151 1408 | 1401 915 | 875    |        |         |
| Naphthalene, 2,6-dimethyl-               | 581-42-0 | 596589  | -              | HC        | polycyclic aromatic HC | 1656 0.52 | 156 1417 | 1416 944 | 932    |        |         |
| Naphthalene, 1,7-dimethyl-               | 24644-78-8 | 310345 | -              | HC        | polycyclic aromatic HC | 1660 0.52 | 156 1420 | 1419 949 | 939    |        |         |
| 4-methyl-1-Indanone                      | 575-37-1  | 763569  | -              | Oxy       | ketone      | 1660 0.855 | 117 1420 | 1444 911 | 908    |        |         |
| 1(3H)-Isobenzofuranone, 5-methyl-        | 54120-64-8 | 101191 | -              | Het       | furan       | 1668 1.065 | 119 1425 | NA 789   | 853    |        |         |
| Germacrene A                             | 28387-44-2 | 231769 | -              | HC        | sesquiterpene | 1674 0.375 | 121 1429 | NA 832   | 852    |        |         |
| 7-Methyl-1-naphthol                      | 6939-33-9  | 104350  | -              | Oxy       | alcohol     | 1676 0.745 | 158 1430 | NA 866   | 815    |        |         |
| Naphthalene, 1,5-dimethyl-               | 26452-86-8 | 914918 | -              | HC        | polycyclic aromatic HC | 1678 0.52 | 156 1432 | 1428 948 | 942    |        |         |
| Benzene, (2-methyl-1-methylenebutyl)-    | 571-61-9  | 136225  | -              | HC        | monocyclic aromatic HC | 1678 0.805 | 132 1432 | NA 780   | 760    |        |         |
| cis-beta-Caryophyllene                   | 550-44-7  | 590520  | -              | HC        | sesquiterpene | 1680 0.32 | 69 1433 | 1431 855 | 858    |        |         |
| N-methylphthalimide                      | 118-65-0  | 136747  | -              | Nit       | imide       | 1680 0.89 | 161 1433 | 1425 924 | 902    |        |         |
| Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-3-(2-propenyl)-, (1a,2a,3a,5a)- | 532-12-7  | 674916  | M              | HC        | alicyclic HC | 1684 0.315 | 81 1435 | NA 784   | 764    |        |         |
| Pyridine, 3-(3,4-dihydro-2H-pyrrol-5-yl)- | 50746-55-9 | 2156822 | -              | Het       | pyridine    | 1684 0.7 | 118 1436 | 1427 935 | 934    |        |         |
| 1,5,9-Decatriene, 2,3,5,8-tetramethyl-   | 230646-72-7 | 442246 | -              | HC        | alkene      | 1686 0.295 | 69 1437 | NA 804   | 802    |        |         |

Continued on next page
| Tentative Identification | CAS     | Peak Area | Health Effects | Class      | Subclass     | $1_{tr}$ (s) | $2_{tr}$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse† | Similarity‡ |
|-------------------------|---------|-----------|----------------|------------|-------------|-------------|-------------|------------|---------|---------|----------|-------------|
| Naphthalene, 1,6-dimethyl- | 575-43-9 | 937384    | X              | HC         | polycyclic aromatic HC | 1686        | 0.515       | 156        | 1437    | 1428    | 895      | 925         |
| Bicyclogermacrene       | 24703-35-3 | 335635   |                | HC         | sesquiterpene | 1688        | 0.355       | 121        | 1438    | NA      | 887      | 885         |
| Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl- | 1985-59-7 | 844734    |                | HC         | polycyclic aromatic HC | 1690        | 0.75        | 145        | 1439    | NA      | 783      | 793         |
| Benzylbenzene           | 101-81-5 | 45621     | X              | HC         | polycyclic aromatic HC | 1692        | 0.435       | 168        | 1441    | 1437    | 859      | 783         |
| 3-Tetradecene, (E)-2,7-Ethanonaph[2,3-b]oxirene, 1a,2,7,7a-tetrahydro-, (1aÁ,2aÁ,7aÁ,7aÁ) | 41446-68-8 | 89482     |                  | HC         | alkene      | 1698        | 0.295       | 69         | 1444    | NA      | 833      | 782         |
| 2-Propyn-1-ol, 3-(4-methylphenyl)- | 54515-76-3 | 290267    | -              | Oxy        | epoxide     | 1700        | 0.405       | 143        | 1446    | NA      | 850      | 773         |
| 2-Indolinone, 1-methyl-trans-beta-Farnesene | 61-70-1 | 60539     | X              | Nit        | aza-arene   | 1700        | 0.87        | 118        | 1446    | NA      | 854      | 786         |
| 3,5-Dimethoxy-4-hydroxytoluene | 07/05/6638 | 448069    |                | HC         | sesquiterpene | 1702        | 0.32        | 93         | 1447    | 1446    | 794      | 812         |
| Germanyacetone          | 3796-70-1 | 2420019   | -              | Oxy        | ketone      | 1704        | 0.57        | 43         | 1448    | 1451    | 928      | 918         |
| cis-beta-Farnesene      | 91-64-5  | 973460    | M              | HC         | sesquiterpene | 1712        | 0.32        | 69         | 1454    | 1452    | 875      | 878         |
| Coumarin                | 28973-97-9 | 182123    | -              | Het        | pyran      | 1712        | 1.12        | 118        | 1454    | 1456    | 886      | 824         |
| Naphthalene, 1,8-dimethyl- | 569-41-5 | 161692    |                | HC         | polycyclic aromatic HC | 1714        | 0.505       | 156        | 1455    | 1450    | 897      | 933         |
| Phenol, 2-methoxy-4-(1-propenyl)-, (Z)- | 5912-86-7 | 783503    | X              | Oxy        | ether      | 1714        | 0.595       | 164        | 1455    | 1441    | 923      | 922         |
| 1,5-Cyclooctadiene, 3-(1-methyl-2-propenyl)- | 16538-88-8 | 507392    | -              | HC         | alicyclic HC | 1718        | 0.32        | 93         | 1457    | NA      | 817      | 787         |

Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)
Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification | CAS   | Peak Area | Health Effects | Class       | Subclass               | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|--------------------------|-------|-----------|----------------|-------------|------------------------|-----------|------------|------------|----------|----------|----------|-------------|
| 1-Tridecanol             | 208-96-8 | 80111     | M              | Oxy alcohol | alcohol                | 1730      | 0.295      | 69         | 1465     | NA       | 800      | 772         |
| Quinoline, 2,4-dimethyl-  | 1198-37-4 | 47591     | -              | Nit aza-arene polycyclic aromatic HC | 1730      | 0.52       | 156        | 1465     | 1472     | 779      | 840         |
| Acenaphthylene           | 112-70-9 | 379721    | X              | HC polycyclic aromatic HC | 1730      | 0.59       | 152        | 1465     | 1466     | 950      | 903         |
| Naphthalene, 1,2,3,5,8,8a-hexahydro- | 62690-65-7 | 307873    | -              | HC polycyclic aromatic HC | 1732      | 0.93       | 134        | 1467     | NA       | 797      | 821         |
| 1,2-Dimethylnaphthalene  | 573-98-8 | 285679    | -              | HC polycyclic aromatic HC | 1734      | 0.525      | 141        | 1468     | 1462     | 850      | 877         |
| Pyridine, 2-phenyl-       | 1008-89-5 | 183106    | M              | Het pyridine | 1736      | 0.57       | 154        | 1469     | 1466     | 833      | 759         |
| 2,6-dimethyl-1H-Indole   | 5649-36-5 | 119974    | -              | Nit aza-arene | 1736      | 0.61       | 144        | 1469     | NA       | 841      | 801         |
| Tetradecane, 3-methyl-    | 18435-22-8 | 54704     | -              | HC alkane | 1738      | 0.28       | 71         | 1470     | 1470     | 839      | 756         |
| Naphthalene, 1,2-dihydro-7-methyl-1-(1-methylethenyl)- | NA | 123546 | - | HC polycyclic aromatic HC | 1738      | 0.41       | 141        | 1470     | NA       | 892      | 762         |
| Alloaromadendrene         | 2189-60-8 | 23610     | -              | HC sesquiterpene monocyclic aromatic HC | 1740      | 0.35       | 161        | 1472     | NA       | 780      | 754         |
| Benzene, octyl-           | 25246-27-9 | 313747    | -              | HC sesquiterpene | 1740      | 0.36       | 92         | 1472     | 1472     | 876      | 813         |
| alpha-Humulene            | 6753-98-6 | 1277858   | -              | HC sesquiterpene | 1742      | 0.32       | 41         | 1473     | 1472     | 833      | 836         |
| Pyridine, 4-phenyl-        | 15158-36-8 | 504920    | -              | Het pyridine | 1744      | 0.61       | 155        | 1474     | 1471     | 915      | 905         |
| 4-Methylphthalaldehyde    | 937-30-4 | 193539    | -              | Oxy aldehyde | 1744      | 1.215      | 119        | 1475     | NA       | 893      | 833         |
| 1H-Inden-1-one, 2,3-dihydro-5,7-dimethyl- | 6682-69-5 | 104103    | -              | Oxy ketone | 1752      | 0.66       | 160        | 1480     | NA       | 885      | 850         |
| Norsolanadione            | NA     | 2661384   | -              | Oxy ketone | 1754      | 1.375      | 43         | 1481     | NA       | 913      | 910         |
| Pyridine, 2-(phenylmethyl)-4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one | 1203-08-3 | 88641     | -              | Het pyridine | 1756      | 0.5        | 168        | 1482     | 1482     | 904      | 835         |
|                           | 101-82-6 | 473512    | X              | Oxy ketone | 1756      | 0.72       | 43         | 1482     | NA       | 887      | 881         |

Continued on next page
| Tentative Identification                          | CAS       | Peak Area | Health Effects | Class      | Subclass | \( t_1 \) (s) | \( t_2 \) (s) | Quant Mass | Exp. RI† | Lib. RI† | Reverse† | Similarity‡ |
|------------------------------------------------|-----------|-----------|----------------|------------|----------|--------------|--------------|------------|----------|----------|----------|-------------|
| Naphthalene, 1,2-dihydro-2,5,8-trimethyl-        | 30316-23-5| 113674    | -              | HC         | polycyclic aromatic HC | 1758   | 0.44       | 157       | 1483     | NA       | 827      | 810         |
| cis-alpha-Farnesene                              | 79756-89-1| 885095    | -              | HC         | sesquiterpene      | 1760   | 0.305      | 93        | 1485     | 1484     | 851      | 863         |
| trans-beta-Ionone                                | 26560-14-5| 43275     | -              | Oxy        | ketone              | 1760   | 0.715      | 177       | 1485     | 1485     | 826      | 796         |
| alpha-Curcumene                                  | 644-30-4  | 109976    | -              | HC         | sesquiterpene      | 1762   | 0.34       | 132       | 1486     | 1486     | 909      | 851         |
| 3-(1-methyl-1H-pyrrol-2-yl)Pyridine              | 487-19-4  | 1779704   | X              | Het        | pyridine            | 1762   | 0.67       | 158       | 1486     | 1488     | 905      | 891         |
| Naphthalene, 1,2-dihydro-1,4,6-trimethyl-        | 55682-80-9| 158080    | -              | HC         | polycyclic aromatic HC | 1764   | 0.43       | 157       | 1487     | NA       | 897      | 870         |
| 5,6-dimethyl-1-Indanone                          | 16440-97-4| 140542    | -              | Oxy        | ketone              | 1766   | 0.675      | 160       | 1489     | NA       | 873      | 884         |
| Benzenamine, N-((1-methyl-2-propynyl)-1-Pentadecene| 53832-62-5| 1222978   | -              | Nit        | amine               | 1768   | 0.565      | 130       | 1490     | NA       | 814      | 823         |
| 5-propionyl-2,3-dihydro-1H-Pyrrolizine           | 13360-61-7| 1143841   | -              | HC         | alkene              | 1770   | 0.29       | 57        | 1491     | 1491     | 925      | 926         |
| 1H-Inden-1-one, 2,3-dihydro-3,4,7-trimethyl-      | 35322-84-0| 77416     | -              | Oxy        | ketone              | 1780   | 0.51       | 153       | 1498     | 1494     | 945      | 922         |
| Pentadecane                                      | 91-55-4   | 4339793   | M              | HC         | alkane              | 1782   | 0.28       | 57        | 1499     | 1500     | 950      | 944         |
| 2,3-dimethyl-1H-Indole                           | 629-62-9  | 688844    | -              | Nit        | aza-arene           | 1782   | 0.64       | 144       | 1499     | 1499     | 925      | 922         |

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**Table S3.** Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification                                      | CAS      | Peak Area | Health Effects | Class       | Subclass            | 1<sub>T<sub>(s) | 2<sub>T<sub>(s) | Quant Mass | Exp. RI<sup>†</sup> | Lib. RI<sup>†</sup> | Reverse<sup>†</sup> | Similarity<sup>‡</sup> |
|----------------------------------------------------------------|----------|-----------|----------------|-------------|---------------------|-----------------|---------------|-------------|----------------|------------------|----------------|-----------------------------|
| Naphthalene, 1-propyl-                                         | 2765-18-6| 126961    | -              | HC          | polycyclic aromatic  | 1784            | 0.49          | 141         | 1500            | 1504             | 867            | 756                         |
| 5',6',7',8'-Tetrahydro-2'-acetonaphthone                        | 774-55-0 | 80865     | -              | Oxy         | ketone              | 1786            | 0.615         | 159         | 1502            | NA               | 793            | 840                         |
| alpha-Farnesene                                                | 4506-36-9| 965150    | -              | HC          | sesquiterpene       | 1790            | 0.32          | 69          | 1504            | 1504             | 936            | 934                         |
| 1,5,8-Trimethyl-1,2-dihydonaphthalene                          | 502-61-4 | 203364    | -              | HC          | polycyclic aromatic  | 1790            | 0.425         | 157         | 1505            | NA               | 775            | 782                         |
| Anthracene, 1,2,3,4,5,6-hexahydro-                             | 613-46-7 | 390324    | M              | HC          | polycyclic aromatic  | 1796            | 0.425         | 128         | 1509            | NA               | 800            | 795                         |
| Naphthalene-2-carbonitrile                                     | 6109-22-4| 129763    | -              | Nit         | nitrile             | 1796            | 0.86          | 153         | 1509            | 1497             | 944            | 839                         |
| beta-Bisabolene                                                | 495-61-4 | 729409    | -              | HC          | sesquiterpene       | 1802            | 0.32          | 69          | 1513            | 1513             | 849            | 850                         |
| 3-methyl-2H-Chromen-2-one                                       | 2445-82-1| 237011    | X              | Het         | pyran               | 1806            | 1             | 131         | 1516            | NA               | 917            | 874                         |
| (1,1'-Biphenyl)-2-amine                                         | 90-41-5  | 65702     | M              | Nit         | amine               | 1808            | 0.595         | 168         | 1517            | NA               | 837            | 758                         |
| 13-Tetradec-11-yn-1-ol                                          | NA       | 48192     | -              | Oxy         | alcohol             | 1822            | 0.305         | 54          | 1527            | 1527             | 807            | 776                         |
| 1H-Pyrazole, 3,5-dimethyl-1-phenyl-                             | 1131-16-4| 614183    | -              | Het         | pyrazole            | 1822            | 0.575         | 171         | 1527            | NA               | 780            | 789                         |
| alpha-Selinene                                                 | 473-13-2 | 508576    | -              | HC          | sesquiterpene       | 1824            | 0.365         | 93          | 1528            | NA               | 845            | 769                         |
| 1-Naphthol                                                     | 90-15-3  | 95804     | X              | Oxy         | alcohol             | 1826            | 0.55          | 144         | 1530            | 1525             | 875            | 758                         |
| Bibenzyl                                                       | 2503-46-0| 392078    | -              | HC          | polycyclic aromatic  | 1828            | 0.44          | 91          | 1531            | 1528             | 931            | 851                         |
| Guiacylacetone                                                 | 103-29-7 | 328662    | -              | Oxy         | ketone              | 1828            | 0.975         | 137         | 1531            | 1532             | 886            | 759                         |
| Dibenzofuran                                                   | 132-64-9 | 316528    | M              | Het         | furan               | 1830            | 0.55          | 168         | 1532            | 1532             | 868            | 843                         |
| Naphthalene, 1,4,5-trimethyl-                                  | 1971-46-6| 244462    | -              | HC          | polycyclic aromatic  | 1836            | 0.5           | 155         | 1537            | 1536             | 935            | 929                         |
| 1H-Indole, 1,2,3-trimethyl-                                    | 2131-41-1| 57556     | -              | Nit         | aza-arene           | 1836            | 0.63          | 158         | 1537            | NA               | 894            | 791                         |
| 1-Phenyl-1-octyne                                              | 16967-02-5| 626540   | -              | HC          | alkyne              | 1846            | 0.41          | 143         | 1543            | NA               | 759            | 759                         |

Continued on next page
| Tentative Identification                                                                 | CAS        | Peak Area | Health Effects | Class       | Subclass             | \( t_{R_1} \) (s) | \( t_{R_2} \) (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|-----------------------------------------------------------------------------------------|------------|-----------|----------------|-------------|----------------------|-------------------|-------------------|------------|---------|---------|---------|------------|
| 2(H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-(R)-                           | 17092-92-1 | 286088    | -              | Oxy         | ketone               | 1846              | 1.685             | 111        | 1544    | 1538    | 895     | 879        |
| Naphthalene, 1,6,7-trimethyl-                                                          | 2245-38-7  | 689027    | -              | HC          | polycyclic aromatic  | 1848              | 0.495             | 155        | 1545    | 1544    | 848     | 846        |
| 2,3'-Dipyridyl                                                                        | 581-50-0   | 2195517   | X              | Het         | pyridine             | 1850              | 0.715             | 155        | 1546    | 1536    | 915     | 900        |
| Aromadendrene                                                                         | 27776-01-8 | 353319    | -              | HC          | sesquiterpene        | 1854              | 0.35              | 105        | 1549    | NA      | 854     | 833        |
| Benzyltoluene                                                                         | 74685-33-9 | 28238     | -              | HC          | polycyclic aromatic  | 1854              | 0.41              | 167        | 1549    | NA      | 844     | 792        |
| 4-Hexadecen-6-yne, (Z)-alpha-Calacorene                                               | 21391-99-1 | 103631    | -              | HC          | alkyne               | 1856              | 0.335             | 69         | 1550    | NA      | 780     | 755        |
| Naphthalene, 1-methyl-7-(1-methylethyl)-                                               | 490-65-3   | 305851    | -              | HC          | polycyclic aromatic  | 1884              | 0.48              | 169        | 1578    | 1578    | 895     | 889        |
| 2,3,7-trimethyl-1H-Indole                                                               | 51766-65-5 | 61397     | -              | Nit         | aza-arene            | 1884              | 0.645             | 158        | 1570    | NA      | 881     | 764        |

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| Tentative Identification | CAS    | Peak Area | Health Effects | Class | Subclass | $t_R$ (s) | Mass Exp. | Lib. RI* | Reverse† Similarity‡ |
|--------------------------|--------|-----------|----------------|-------|----------|----------|-----------|----------|---------------------|
| gamma-Dehydro-ar-himachalene | 62235-06-7 | 116474 | - | HC | sesquiterpene | 1888 | 0.405 | 157 | 1573 | NA | 809 | 756 |
| (3E,7E)-4,8,12-Trimethyltrideca-1,3,7,11-tetraene | 1081-77-2 | 684188 | - | HC | alkene | 1890 | 0.32 | 69 | 1574 | 1573 | 889 | 889 |
| Benzene, nonyl- | 5037-60-5 | 327963 | - | HC | monocyclic aromatic | 1892 | 0.36 | 92 | 1575 | 1576 | 939 | 885 |
| 1H-Phenalene | 203-80-5 | 312105 | - | HC | polycyclic aromatic | 1902 | 0.58 | 165 | 1582 | 1583 | NA | 888 | 852 |
| 1H-Inden-1-one, 2,3-dihydro-4,7-dimethyl- | 212394-95-1 | 137442 | - | Oxy | ketone | 1902 | 0.85 | 117 | 1583 | NA | 889 | 849 |
| Eudesma-1,4(15),11-triene | 229-934-9 | 46115 | X | HC | sesquiterpene | 1908 | 0.36 | 108 | 1586 | NA | 804 | 752 |
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 525-40-6 | 426073 | - | Oxy | ester | 1912 | 0.635 | 71 | 1589 | 1588 | 846 | 804 |
| 1H-Pyrido[3,4-b]indole, 2,3,4,9-tetrahydro-1-methyl-1-Hexadecene | 629-73-2 | 133515 | - | Nit | aza-arene | 1914 | 0.545 | 171 | 1591 | NA | 796 | 786 |
| Hexadecane | 14002-89-2 | 483957 | - | HC | alkene | 1916 | 0.29 | 83 | 1592 | 1592 | 929 | 930 |
| 2H-1-Benzopyran-2-one, 4,6-dimethyl- | 21296-92-4 | 56117 | M | Oxy | ketone | 1920 | 0.87 | 145 | 1595 | NA | 796 | 855 |
| Hexadecane | 6627-88-9 | 1189451 | - | HC | alkane | 1926 | 0.28 | 57 | 1599 | 1600 | 933 | 929 |
| 1H-Indole, 2,3,5-trimethyl- | 544-76-3 | 161784 | X | Nit | aza-arene | 1926 | 0.6 | 158 | 1599 | 1593 | 922 | 838 |
| Methoxyeugenol | 86-73-7 | 34186 | G3 | Oxy | ether | 1926 | 0.62 | 194 | 1599 | 1602 | 850 | 798 |
| Fluorene | 613-33-2 | 869220 | - | HC | polycyclic aromatic | 1928 | 0.54 | 166 | 1600 | 1606 | 921 | 921 |
| 4,4'-Dimethylbiphenyl | 1855-47-6 | 120985 | - | HC | polycyclic aromatic | 1942 | 0.455 | 182 | 1611 | 1608 | 904 | 869 |

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Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification | CAS       | Peak Area | Health Effects | Class   | Subclass      | $t_R$ (s) | $t_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse† | Similarity‡ |
|--------------------------|-----------|-----------|----------------|---------|---------------|-----------|-----------|------------|--------|--------|----------|-------------|
| 1-Isopropenynaphthalene  | 2523-37-7 | 138619    | -              | HC      | polycyclic    | 1948      | 0.515     | 153        | 1615   | NA     | 831      | 815         |
| 9-methyl-9H-Fluorene     | 4854-85-7 | 225786    | -              | HC      | polycyclic    | 1954      | 0.51       | 165        | 1620   | 1579   | 904      | 895         |
| trans-p-Dimethylaminocinnaminitril | 92-83-1 | 218938    | -              | Nit     | nitrile       | 1956      | 0.655     | 171        | 1621   | NA     | 801      | 763         |
| 9H-Xanthene               | 119-61-9 | 88395     | G2B            | Het     | pyran         | 1978      | 0.515     | 181        | 1638   | 1635   | 913      | 769         |
| 1,4,5,8-Tetramethynaphthalene | 2717-39-7 | 134399    | -              | HC      | polycyclic    | 1984      | 0.475     | 169        | 1642   | NA     | 810      | 846         |
| Benzophenone              | 14002-90-5| 79281     | -              | Oxy     | ketone        | 1984      | 0.665     | 105        | 1642   | 1644   | 937      | 769         |
| 4,7-Dimethylcoumarin      | 3892-00-0 | 107391    | -              | Het     | pyran         | 1984      | 0.975     | 145        | 1643   | NA     | 893      | 815         |
| Pentadecane, 2,6,10-trimethyl- | 34318-21-3 | 620107 | -              | HC      | alkane        | 1990      | 0.29       | 57         | 1647   | 1649   | 901      | 901         |
| 1,4-Naphthalenedione, 2,3-dimethyl- | 2197-57-1 | 84109     | X              | Oxy     | ketone        | 1996      | 0.735     | 186        | 1651   | NA     | 863      | 837         |
| 2-Cyclobexen-1-one, 4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl- | 610-35-5 | 840376    | -              | Oxy     | ketone        | 1996      | 1.16       | 108        | 1652   | 1648   | 899      | 890         |
| 4-Hydroxyphthalate        | 229-95-8 | 174422    | -              | Oxy     | ester         | 2000      | 0.545     | 181        | 1654   | NA     | 905      | 821         |
| 6H-Dibenz[o][b,d]-pyran   | 629-74-3 | 37063     | -              | Het     | pyran         | 2012      | 0.54       | 181        | 1663   | NA     | 793      | 875         |
| 1-Hexadecyne              | 16369-12-3| 95723     | -              | HC      | alkene        | 2024      | 0.29       | 54         | 1672   | NA     | 868      | 899         |
| 8-Heptadecene             | NA       | 303858    | -              | HC      | alkene        | 2034      | 0.29       | 69         | 1679   | 1679   | 878      | 887         |
| Decylbenzene              | 104-72-3 | 154950    | X              | HC      | monocyclic    | 2036      | 0.355     | 92         | 1681   | 1681   | 837      | 799         |
| Propanedinitrile, 2-(2,2,3,4-tetramethyl-4-cyclopenten-1-ylidene) | 3031-15-0 | 202415    | -              | Nit     | nitrile       | 2036      | 0.555     | 171        | 1681   | NA     | 789      | 773         |

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| Tentative Identification | CAS    | Peak Area | Health Effects | Class       | Subclass      | $t_1R$ (s) | $t_2R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse† | Similarity‡ |
|-------------------------|--------|-----------|----------------|-------------|---------------|------------|------------|------------|---------|---------|----------|-------------|
| Naphthalene, 1,2,3,4-tetramethyl- | 2040-10-0 | 66877     | -              | HC          | polycyclic aromatic HC | 2040 | 0.5 | 169 | 1684 | NA | 837 | 780 |
| 4’-tert-Butyl-2′,6′-dimethylacetophenone | 6765-39-5 | 191140    | -              | Oxy         | ketone        | 2046 | 0.485 | 189 | 1688 | NA | 837 | 792 |
| 1-Heptadecene           | 2345-28-0 | 418702    | -              | HC          | alkene        | 2052 | 0.29  | 57  | 1693 | 1693 | 925 | 933 |
| 2-Pentadecanone         | 629-78-7  | 125015    | -              | Oxy         | ketone        | 2060 | 0.53  | 58  | 1699 | 1699 | 781 | 877 |
| Heptadecane             | 20675-95-0 | 1230578   | -              | HC          | alkane        | 2062 | 0.28  | 57  | 1700 | 1700 | 952 | 937 |
| (E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol | 1430-97-3 | 82807     | -              | Oxy         | ether         | 2068 | 0.635 | 194 | 1705 | 1704 | 894 | 865 |
| 9H-Fluorene, 2-methyl-   | 36151-02-7 | 49239     | -              | HC          | polycyclic aromatic HC | 2074 | 0.565 | 180 | 1710 | 1720 | 822 | 770 |
| Blumenol C              | 1556-99-6  | 36793     | -              | Oxy         | alcohol       | 2078 | 1.175 | 108 | 1713 | 1713 | 870 | 784 |
| 4-methyl-9H-fluorene    | 486-56-6   | 800705    | X              | HC          | polycyclic aromatic HC | 2084 | 0.525 | 165 | 1717 | NA | 891 | 895 |
| Cotinine                | 62600-05-9  | 774111    | -              | Het         | pyrrole       | 2084 | 1.34  | 98  | 1718 | NA | 938 | 930 |
| Cedran-diol, 8S,14-     | 3910-35-8  | 621536    | -              | Oxy         | alcohol       | 2086 | 0.59  | 43  | 1719 | NA | 788 | 768 |
| 1H-Indene, 2,3-dihydro-1,1,3-trimethyl-3-phenyl- | 1730-37-6 | 72676     | -              | HC          | polycyclic aromatic HC | 2092 | 0.41  | 143 | 1723 | 1714 | 792 | 765 |
| 9H-Fluorene, 1-methyl-   | 4569-45-3   | 330566    | M              | HC          | polycyclic aromatic HC | 2094 | 0.55  | 165 | 1725 | 1719 | 953 | 926 |
| 9H-Fluorene, 9,9-dimethyl- | 529-05-5   | 192044    | X              | HC          | polycyclic aromatic HC | 2102 | 0.5   | 179 | 1731 | NA | 881 | 824 |
| Chamazulene             | 24875-94-3  | 86785     | -              | HC          | polycyclic aromatic HC | 2106 | 0.515 | 169 | 1734 | 1734 | 806 | 848 |
| 6’-Methyl-2’-acetonaphthone | 2980-70-3  | 36967     | -              | Oxy         | ketone        | 2114 | 0.765 | 169 | 1741 | NA | 882 | 787 |

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| Tentative Identification                                      | CAS     | Peak Area | Health Effects | Class | Subclass | $1_{R}$ (s) | $2_{R}$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|---------------------------------------------------------------|---------|-----------|----------------|-------|----------|-------------|-------------|------------|----------|----------|----------|-------------|
| Cyclopentane, 1,1'-((1,4-butandiyl)bis-| 20071-09-4 | 74995     |                | HC    | alicyclic | 2138        | 0.305       | 67         | 1759     | NA       | 789      | 781        |
| Benzene, 1,1'-((1,2-cyclobutanediyl)bis-, trans-            | 486-25-9 | 379014    |                | HC    | monocyclic | 2140        | 0.44        | 104        | 1760     | NA       | 885      | 869        |
| 9H-Fluroen-9-one                                             | 20490-42-0 | 99389     |                | Oxy   | ketone    | 2144        | 0.755       | 180        | 1764     | 1752     | 932      | 821        |
| 1,4-Naphthalenedione, 2,3,6-trimethyl-                      | 7206-15-7 | 179303    |                | Oxy   | ketone    | 2164        | 0.73        | 200        | 1779     | NA       | 893      | 878        |
| (3E)-3-Octadecene                                            | 593-45-3 | 404442    |                | HC    | alkenes   | 2184        | 0.29        | 55         | 1794     | 1795     | 900      | 904        |
| Octadecane                                                   | 18787-63-8 | 506640    |                | HC    | alkenes   | 2192        | 0.28        | 57         | 1800     | 1800     | 936      | 928        |
| 2-Hexadecanone                                               | 85-01-8  | 170462    | G3             | Oxy   | ketone    | 2192        | 0.515       | 58         | 1800     | 1800     | 929      | 895        |
| Phenanthrene                                                 | 37841-91-1 | 327195    | M              | HC    | polycyclic | 2200        | 0.61        | 178        | 1807     | 1797     | 942      | 935        |
| Isovelleral                                                   | 54878-25-0 | 69041     |                | Oxy   | aldehyde  | 2204        | 0.73        | 91         | 1810     | NA       | 799      | 783        |
| Solavetivone                                                  | 120-12-7 | 54695     | G3             | Oxy   | ketone    | 2214        | 0.93        | 108        | 1819     | NA       | 919      | 849        |
| Anthracene                                                   | 4612-63-9 | 101304    |                | HC    | polycyclic | 2216        | 0.61        | 178        | 1820     | 1817     | 928      | 835        |
| 9H-Fluorene, 2,3-dimethyl-                                   | 504-96-1 | 213165    |                | HC    | polycyclic | 2234        | 0.535       | 179        | 1835     | NA       | 803      | 907        |
| Neophytadiene                                                | 17239-99-5 | 12532161  |                | HC    | diterpene | 2240        | 0.33        | 68         | 1840     | 1840     | 938      | 925        |
| Anthracene, 9,10-dihydro-9-methyl-                           | 2437-93-6 | 63867     |                | HC    | polycyclic | 2240        | 0.52        | 178        | 1840     | NA       | 763      | 810        |
| 2-Phytene (trans)                                            | 629-89-0  | 764375    |                | HC    | alkenes   | 2244        | 0.3         | 70         | 1843     | 1838     | 873      | 870        |
| 1-Octadecyne                                                 | 502-69-2  | 38040     |                | HC    | alkyne    | 2244        | 0.31        | 123        | 1843     | NA       | 803      | 787        |
| 2-Pentadecanone, 6,10,14-trimethyl-                          | 2854-40-2 | 879160    |                | Oxy   | ketone    | 2244        | 0.53        | 58         | 1843     | 1844     | 892      | 857        |
| Cyclo(L-prolyl-L-valine)                                     | 942-43-8  | 57422     |                | Nit   | amino acid | 2262        | 1.31        | 70         | 1859     | NA       | 856      | 766        |

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Table S3. Tentatively identified compounds from the particulate phase fraction of mainstream tobacco smoke (Continued)

| Tentative Identification | CAS       | Peak Area | Health Effects | Class         | Subclass            | $t_R$ (s) | 2$^	ext{nd}$ $t_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse$^1$ | Similarity$^1$ |
|--------------------------|-----------|-----------|----------------|---------------|---------------------|----------|-------------------------|------------|--------|--------|-------------|----------------|
| Anthracene, 9,10-dihydro-2-methyl- | 244-99-5  | 87506     | -              | HC            | polycyclic aromatic HC | 2268     | 0.525                  | 179        | 1863   | NA     | 841         | 780            |
| 4-Azafluorene            | NA        | 99321     | -              | Nit           | aza-arene           | 2274     | 0.675                  | 167        | 1868   | NA     | 888         | 777            |
| 3,7,11-Trimethyl-2,4-dodecadiene | 67858-77-9 | 110144    | -              | HC            | alkene              | 2288     | 0.31                   | 82         | 1879   | NA     | 785         | 769            |
| 4,8,12-Tetradecatrien-1-ol, 5,9,13-trimethyl- | 18435-45-5 | 70755     | -              | Oxy           | alcohol             | 2304     | 0.305                  | 69         | 1892   | NA     | 823         | 785            |
| 1-Nonadecene            | 629-92-5  | 107088    | -              | HC            | alkene              | 2306     | 0.3                    | 83         | 1894   | 1894   | 914         | 927            |
| Nonadecane              | NA        | 368271    | -              | HC            | alkene              | 2314     | 0.28                   | 57         | 1900   | 1900   | 911         | 934            |
| 3-hydroxy-Solvavetivone | 2922-51-2 | 74626     | -              | Oxy           | ketone              | 2314     | 0.84                   | 108        | 1901   | NA     | 777         | 753            |
| 2-Heptadecanone         | 70901-63-2 | 245750    | -              | Oxy           | ketone              | 2316     | 0.51                   | 58         | 1902   | 1902   | 930         | 894            |
| beta-Springene          | 01/11/7557 | 271655    | -              | HC            | alkene              | 2330     | 0.32                   | 69         | 1914   | NA     | 872         | 863            |
| trans,trans-Farnesyl acetone | 832-69-9  | 596314    | G3             | Oxy           | ketone              | 2330     | 0.515                  | 43         | 1914   | 1914   | 885         | 883            |
| Phenanthrene, 1-methyl- | 112-39-0  | 32942     | -              | HC            | polycyclic aromatic HC | 2340     | 0.615                  | 192        | 1924   | 1934   | 912         | 787            |
| Hexadecanoic acid, methyl ester | 613-12-7  | 479573    | M              | Oxy           | ester               | 2344     | 0.41                   | 74         | 1926   | 1926   | 945         | 892            |
| Anthracene, 2-methyl-   | 610-48-0  | 75571     | -              | HC            | polycyclic aromatic HC | 2348     | 0.615                  | 192        | 1929   | 1928   | 940         | 865            |
| Anthracene, 1-methyl-   | 123-69-3  | 32834     | X              | HC            | polycyclic aromatic HC | 2362     | 0.615                  | 192        | 1941   | 1935   | 793         | 905            |
| Oxacycloheptadec-8-en-2-one | 19943-27-2 | 155135    | -              | Oxy           | ketone              | 2366     | 0.56                   | 67         | 1945   | 1936   | 867         | 846            |
| Cycro-(Pro-Pro)         | 1898-13-1 | 260070    | -              | Nit           | amino acid          | 2378     | 1.23                   | 70         | 1955   | NA     | 925         | 837            |
| (+)-Cembrene            | 77898-97-6 | 386081    | -              | HC            | alicyclic HC        | 2380     | 0.38                   | 91         | 1956   | NA     | 864         | 830            |
| alpha-Springene         | 74685-27-1 | 359823    | -              | HC            | alkene              | 2390     | 0.32                   | 69         | 1965   | 1969   | 882         | 871            |
| Tentative Identification | CAS     | Peak Area | Health Effects | Class | Subclass | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI$^*$ | Lib. RI$^*$ | Reverse$^†$ | Similarity$^‡$ |
|--------------------------|---------|-----------|----------------|-------|----------|-----------|------------|------------|-------------|-------------|-------------|-------------|
| 3-Eicosene, (E)-         | 112-95-8 | 89467     |                | HC    | alkene   | 2424      | 0.3        | 57         | 1994        | NA          | 877         | 900         |
| Eicosane                 | 5508-58-7 | 198869    | M              | HC    | alkane   | 2432      | 0.29       | 57         | 2000        | 2000        | 917         | 904         |
| Andrographolide          | 29837-07-8 | 72113     |                | Oxy   | alcohol  | 2472      | 0.44       | 91         | 2036        | NA          | 834         | 784         |
| cis-alpha-Bisabolene epoxide | 948-67-4 | 766502    |                | Oxy   | epoxide  | 2534      | 0.505      | 43         | 2092        | NA          | 786         | 780         |
| 10-Heneicosene (c,t)     | 629-94-7 | 52730     |                | HC    | alkene   | 2538      | 0.305      | 57         | 2095        | NA          | 861         | 895         |
| Heneicosane              | 150-86-7 | 149168    |                | HC    | alkane   | 2544      | 0.3        | 57         | 2100        | 2100        | 912         | 888         |
| Phytol                   | 629-97-0 | 125892    |                | Oxy   | alcohol  | 2560      | 0.42       | 71         | 2116        | 2116        | 888         | 808         |
| Docosane                 | 107304-12-1 | 127122   |                | HC    | alkane   | 2650      | 0.3        | 57         | 2200        | 2200        | 892         | 842         |
| Stig mastan-6,22-dien, 3,5-dedihydro- | 10191-41-0 | 111497    |                | HC    | triterpene | 3424    | 0.695      | 81         | 2945        | NA          | 832         | 816         |
| Vitamin E                | 64-19-7 | 1523058   |                | Oxy   | alcohol  | 3504      | 0.78       | 165        | 3022        | NA          | 856         | 855         |

$^*$RI is Kovats Retention Index. “Exp. RI” refers to an experimental retention index calculated for this analysis. “Library RI” refers to a tabulated RI value obtained from NIST, PubChem, or ChemSpider electronic sources.

$^†$Similarity refers to a “forward” mass spectral match score (i.e., how well does an experimentally-obtained spectrum fit to a library entry). In the case of a forward search, the match score (out of a maximum of 1000) for the experimental spectrum is penalized for containing extra peaks that are not present in the library spectrum.

$^‡$Reverse refers to a “backwards” mass spectral match score (i.e., how well does a library entry fit to an experimentally-obtained spectrum). A reverse search match score (out of a maximum of 1000) for the library spectrum is not penalized for having extra peaks not contained in the experimental spectrum. A reverse search only requires that peaks in the library spectrum are present in the experimental spectrum.

Health effects were classified using the International Agency for Research on Cancer (IARC) carcinogen list and the Registry of Toxic Effects of Chemical Substances (RTECS) provided by the Canadian Centre for Occupational Health and Safety (CCOHS).

G1 = Group 1 carcinogen, G2A = Group 2A carcinogen, G2B = Group 2B carcinogen, G3 = Group 3 carcinogen, M = mutagen, T = teratogen, X = toxic by other mechanisms, “–” = no risk data available/risks mitigated by proper protective equipment.

NA = not available, HC = hydrocarbon, Het = heterocycle, Misc = miscellaneous, Nit = nitrogenated, Oxy = oxygenated
Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke. G1 = Group 1 carcinogen, G2A = Group 2A carcinogen, G2B = Group 2B carcinogen, G3 = Group 3 carcinogen, M = Mutagen, T = Teratogen, X = Toxic by other mechanisms, ND = No risk data available or risks mitigated by proper protective equipment.

| Tentative Identification | CAS     | Peak Area | Health Effects | Class       | Subclass                  | $t_R (s)$ | $t_R (s)$ | Quant Mass | Exp. RI$^*$ | Lib. RI$^*$ | Reverse† | Similarity‡ |
|--------------------------|---------|-----------|----------------|-------------|---------------------------|----------|----------|------------|-------------|-------------|----------|-------------|
| Acetic acid              | 64-19-7 | 12425147  | -              | Oxy         | carboxylic acid           | 224      | 0.35     | 60         | 650         | 645         | 978      | 978         |
| 3-methyl-2-butanone      | 563-80-4 | 83823     | -              | Oxy         | ketone                   | 224      | 0.45     | 86         | 650         | 653         | 909      | 909         |
| 2-methyl-butanal         | 96-17-3 | 82376     | -              | Oxy         | aldehyde                 | 274      | 0.59     | 58         | 681         | 681         | 946      | 822         |
| Butanenitrile            | 109-74-0 | 475077    | X              | Nit         | nitrile                  | 282      | 0.965    | 41         | 686         | 686         | 955      | 899         |
| (2E)-2-Butenenitrile     | 4786-20-3 | 841321    | -              | Nit         | nitrile                  | 296      | 1.05     | 41         | 695         | 697         | 963      | 889         |
| 2-Pentanone              | 107-87-9 | 508247    | -              | Oxy         | ketone                   | 296      | 0.78     | 43         | 694         | 691         | 954      | 875         |
| Methyl thiocyanate       | 556-64-9 | 459740    | X              | Misc        | thiocyanate              | 330      | 0.94     | 72         | 715         | 711         | 956      | 935         |
| Butanenitrile, 2-methyl- | 18936-17-9 | 1176152   | X              | Nit         | nitrile                  | 342      | 1.1      | 55         | 723         | 717         | 937      | 934         |
| Butanenitrile, 3-methyl- | 625-28-5 | 2487831   | X              | Nit         | nitrile                  | 352      | 1.14     | 43         | 729         | 731         | 909      | 908         |
| Pyrazine                 | 290-37-9 | 1582045   | M              | Het         | pyrazine                 | 358      | 0.625    | 80         | 732         | 734         | 968      | 968         |
| 1H-Pyrrole, 1-methyl-     | 96-54-8 | 737950    | -              | Het         | pyrrole                  | 364      | 0.64     | 80         | 736         | 735         | 917      | 895         |
| 4-methyl-2-pentanone     | 108-10-1 | 235009    | -              | Oxy         | ketone                   | 364      | 0.87     | 43         | 736         | 736         | 915      | 838         |
| 3-Penten-2-one, (E)-     | 3102-33-8 | 287355    | X              | Oxy         | ketone                   | 368      | 1.045    | 69         | 738         | 739         | 946      | 789         |
| Pyridine                 | 110-86-1 | 9542703   | G2B            | Het         | pyridine                 | 372      | 0.665    | 79         | 741         | 740         | 941      | 941         |
| (Dimethylamino)-acetonitrile | 926-64-7 | 249399    | X              | Nit         | nitrile                  | 380      | 1.035    | 83         | 746         | NA          | 922      | 897         |
| Pyrrole                  | 109-97-7 | 7104916   | M              | Het         | pyrrole                  | 384      | 0.57     | 67         | 748         | 748         | 979      | 979         |
| 1,3,5-Cycloheptatriene   | 544-25-2 | 55934     | M              | HC          | alicyclic HC             | 412      | 0.46     | 65         | 765         | 765         | 944      | 926         |
| 3,3-Dimethylacrylonitrile | 4786-24-7 | 786277    | -              | Nit         | nitrile                  | 422      | 1.285    | 41         | 772         | 770         | 889      | 857         |
| Pentenitrile             | 110-59-8 | 343324    | X              | Nit         | nitrile                  | 428      | 1.21     | 54         | 775         | 777         | 915      | 858         |
| 3-Hexanone               | 589-38-8 | 87638     | M              | Oxy         | ketone                   | 442      | 0.81     | 57         | 783         | 783         | 944      | 782         |
| 2-Hexanone               | 591-78-6 | 127877    | M              | Oxy         | ketone                   | 450      | 0.92     | 58         | 788         | 789         | 919      | 825         |
| Cyclopentanone           | 120-92-3 | 1640759   | -              | Oxy         | ketone                   | 454      | 1.055    | 55         | 791         | 791         | 980      | 974         |
| 1H-Pyrrole, 1-ethyl-      | 617-92-5 | 310687    | -              | Het         | pyrrole                  | 494      | 0.655    | 80         | 812         | 811         | 909      | 896         |
| 2-Methylpyridine         | 109-06-8 | 1797843   | M              | Het         | pyridine                 | 502      | 0.61     | 93         | 815         | 815         | 953      | 944         |
Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke (Continued)

| Tentative Identification | CAS     | Peak Area | Health Effects | Class  | Subclass | mass | Exp. RI | Lib. RI | Reverse † | Similarity ‡ |
|--------------------------|---------|-----------|----------------|--------|----------|------|--------|---------|-----------|--------------|
| 2-Methylpyrazine         | 109-08-0| 43935969  | M              | Het    | pyrazine | 520  | 0.66   | 94      | 824       | 824          | 970          | 970          |
| 2-Cyclopenten-1-one      | 930-30-3| 2122603   | -              | Oxy    | ketone   | 538  | 1.25   | 82      | 833       | 832          | 959          | 952          |
| 4,4-Dimethyl-3-            | 59997-51-2| 1228765             | X        | Nit    | nitrile  | 550  | 1.23   | 57      | 838       | 843          | 765          | 755          |
| Oxopentanenitrile        |         |           |                |        |          |      |        |         |           |              |              |              |
| Pentanenitrile, 4-methyl-| 542-54-1| 3485465   | -              | Nit    | nitrile  | 556  | 1.27   | 55      | 841       | 843          | 920          | 920          |
| Cyclopentanone, 2-methyl- | 1120-72-5| 329084      | -              | Oxy    | ketone   | 556  | 0.955  | 42      | 841       | 840          | 949          | 910          |
| 2-Hexanone, 4-methyl-     | 105-42-0| 70851     | -              | Oxy    | ketone   | 566  | 0.915  | 58      | 846       | 846          | 919          | 802          |
| Cyclopentanone, 3-methyl- | 1757-42-2| 150877     | -              | Oxy    | ketone   | 574  | 1.08   | 69      | 850       | 851          | 924          | 868          |
| 5-methyl-2-hexanone      | 110-12-3| 396962    | -              | Oxy    | ketone   | 588  | 0.945  | 43      | 856       | 857          | 943          | 899          |
| 2-Furanmethanol          | 98-00-0 | 973987    | G2B            | Het    | furan    | 590  | 0.65   | 98      | 857       | 858          | 954          | 939          |
| Ethylbenzene             | 100-41-4| 2234959   | G2B            | HC     | monocyclic aromatic HC | 600 | 0.46   | 91      | 862       | 860          | 952          | 952          |
| Pyridine, 3-methyl-      | 108-99-6| 1048871   | M              | Het    | pyridine | 602  | 0.79   | 93      | 863       | 863          | 952          | 941          |
| 2-Propanone, 1-(acetyloxy)- | 592-20-1| 12941977 | -              | Oxy    | ketone   | 608  | 1.485  | 43      | 866       | 867          | 970          | 948          |
| m-Xylene                 | 108-38-3| 2852196   | G3             | HC     | monocyclic aromatic HC | 618 | 0.465  | 91      | 870       | 870          | 957          | 957          |
| o-Xylene                 | 95-47-6 | 52148     | G3             | HC     | monocyclic aromatic HC | 630 | 0.465  | 91      | 876       | 876          | 925          | 855          |
| Phenylethyne             | 536-74-3| 308920    | X              | HC     | monocyclic aromatic HC | 636 | 0.51   | 102     | 879       | 877          | 927          | 896          |
| Hexanenitrile            | 628-73-9| 473963    | X              | Nit    | nitrile  | 636  | 1.195  | 54      | 879       | 879          | 928          | 905          |
| Pyridine, 2,6-dimethyl-   | 108-48-5| 207125    | M              | Het    | pyridine | 642  | 0.505  | 107     | 881       | 880          | 914          | 851          |
| 1,5-Heptadiene, 2,6-dimethyl- | 6709-39-3| 140490 | -              | HC     | alkene   | 644  | 0.345  | 69      | 882       | 882          | 888          | 834          |
| 2-heptanone              | 110-43-0| 604107    | M              | Oxy    | ketone   | 660  | 0.88   | 58      | 890       | 890          | 930          | 928          |
| 1-nonene                 | 124-11-8| 58573     | -              | HC     | alkene   | 662  | 0.345  | 56      | 891       | 890          | 913          | 837          |
Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke (Continued)

| Tentative Identification | CAS     | Peak Area | Health Effects | Class | Subclass | \( t_R \) (s) | Quant Mass | Exp. RI | Lib. RI | Reverse† | Similarity‡ |
|--------------------------|---------|-----------|----------------|-------|----------|-------------|------------|--------|--------|----------|------------|
| Styrene                  | 100-42-5| 3579752   | G2A            | HC    | monocyclic aromatic | 666 | 0.5 | 104 | 893 | 894 | 952 | 952 |
| p-Xylene                 | 106-42-3| 1052166   | G3             | HC    | monocyclic aromatic | 668 | 0.485 | 91 | 894 | 894 | 944 | 942 |
| Cyclohexanone            | 108-94-1| 99791     | G3             | Oxy   | ketone       | 674 | 1.045 | 55 | 897 | 896 | 922 | 811 |
| Annulene                 | 629-20-9| 139454    | -              | HC    | monocyclic aromatic | 682 | 0.51 | 104 | 900 | 894 | 900 | 802 |
| Nonane                   | 111-84-2| 57625     | X              | HC    | alkane       | 682 | 0.33 | 57 | 900 | 900 | 939 | 864 |
| 3-Methylcyclopentyl acetate | 24070-70-0 | 162858 | -             | Oxy   | ester       | 684 | 0.56 | 43 | 901 | 904 | 867 | 796 |
| Pyridine, 2-ethyl-       | 100-71-0| 407090    | -              | Het   | pyridine     | 690 | 0.545 | 106 | 904 | 904 | 910 | 886 |
| 2-Cyclopenten-1-one, 2-methyl- | 1120-73-6 | 2089619 | -             | Oxy   | ketone       | 694 | 1.015 | 67 | 906 | 905 | 961 | 959 |
| Furfuryl formate         | 13493-97-5| 122285 | -             | Oxy   | ester       | 698 | 0.755 | 81 | 908 | 904 | 952 | 848 |
| 2-Acetyl furan           | 1192-62-7| 2597557   | M              | Het   | furan        | 708 | 1.035 | 95 | 912 | 911 | 941 | 940 |
| Pyrazine, 2,6-dimethyl-  | 108-50-9| 1646230   | M              | Het   | pyrazine     | 710 | 0.595 | 108 | 913 | 913 | 945 | 932 |
| Pyrazine, 2,5-dimethyl-  | 123-32-0| 279855    | M              | Het   | pyrazine     | 716 | 0.59 | 42 | 916 | 915 | 912 | 849 |
| Pyrazine, ethyl-         | 13925-00-3| 673428 | M              | Het   | pyrazine     | 718 | 0.6  | 107 | 917 | 917 | 961 | 948 |
| Anisole                  | 100-66-3| 447452    | -              | Oxy   | ether        | 722 | 0.57 | 65 | 919 | 918 | 929 | 846 |
| 2,3-dimethylpyrazine     | 5910-89-4| 925690    | X              | Het   | pyrazine     | 722 | 0.61 | 67 | 919 | 919 | 929 | 905 |
| Cumene                   | 98-82-8| 142922    | G2B            | HC    | monocyclic aromatic | 736 | 0.455 | 105 | 925 | 925 | 952 | 914 |
| alpha-Thujene            | 02/05/2867| 156090 | -              | HC    | monoterpane  | 744 | 0.35 | 93 | 929 | 929 | 913 | 891 |
| 2,4-dimethylpyridine     | 108-47-4| 259182    | M              | Het   | pyridine     | 754 | 0.625 | 106 | 933 | 932 | 934 | 861 |
| Pyrazine, ethenyl-       | 4177-16-6| 215011   | -              | Het   | pyrazine     | 760 | 0.61 | 106 | 936 | 935 | 845 | 800 |
| alpha-Pinene             | 80-56-8| 322423    | -              | HC    | monoterpen   | 760 | 0.365 | 55 | 936 | 927 | 916 | 914 |
| 2-methylcyclohexanone    | 583-60-8| 41977     | X              | Oxy   | ketone       | 772 | 0.89 | 84 | 942 | 937 | 802 | 714 |

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| Tentative Identification                  | CAS      | Peak Area | Health Effects | Class     | Subclass       | 1<sub>r</sub> (s) | 2<sub>r</sub> (s) | Quant Mass | Exp. RI† | Lib. RI† | Reverse† | Similarity‡ |
|------------------------------------------|----------|-----------|----------------|-----------|----------------|-------------------|------------------|-------------|----------|----------|----------|------------|
| Pyridine, 2,3-dimethyl-                  | 583-61-9 | 176593    | M              | Het       | pyridine       | 780               | 0.63             | 106         | 945      | 945      | 927      | 873        |
| Benzene, 2-propenyl-                     | 300-57-2 | 275674    | X              | HC        | monocyclic aromatic | 786               | 0.45             | 117         | 948      | 947      | 936      | 926        |
| Camphene                                 | 79-92-5  | 225909    | -              | HC        | monoterpene    | 798               | 0.38             | 93          | 953      | 954      | 950      | 930        |
| Benzene, propyl-                         | 103-65-1 | 1587107   | -              | HC        | monocyclic aromatic | 804               | 0.44             | 91          | 956      | 956      | 978      | 946        |
| Cyclopentanone, 3,4-bis(methylene)-      | 27646-73-7 | 146127    | -              | Oxy       | ketone         | 812               | 0.88             | 79          | 959      | 949      | 850      | 764        |
| 3-Ethyltoluene                           | 620-14-4 | 1359132   | -              | HC        | monocyclic aromatic | 820               | 0.445            | 105         | 964      | 963      | 944      | 943        |
| 3,3-dimethylacrylic acid                 | 541-47-9 | 115096    | -              | Oxy       | carboxylic acid| 822               | 0.545            | 83          | 964      | 953      | 831      | 745        |
| 2-Ethyltoluene                           | 611-14-3 | 1364376   | -              | HC        | monocyclic aromatic | 826               | 0.425            | 105         | 966      | 967      | 938      | 938        |
| 3-methyl-2-cyclopenten-1-one             | 2758-18-1 | 829456    | -              | Oxy       | ketone         | 828               | 1.38             | 96          | 968      | 969      | 941      | 925        |
| Benzoaldehyde                            | 100-52-7 | 142955    | M              | Oxy       | aldehyde       | 830               | 0.84             | 106         | 968      | 970      | 905      | 798        |
| 1,2,4-trimethylbenzene                   | 95-63-6  | 573435    | M              | HC        | monocyclic aromatic | 838               | 0.435            | 105         | 972      | 976      | 940      | 939        |
| Dimethyl trisulfide                      | 3658-80-8 | 101042    | -              | Misc      | trisulfide     | 840               | 0.485            | 126         | 973      | 973      | 916      | 878        |
| (R)-Sabinene                             | 3387-41-5 | 336230    | -              | HC        | monoterpene    | 848               | 0.385            | 93          | 976      | 976      | 929      | 911        |
| Methyl 2-furoate                         | 611-13-2 | 315709    | -              | Oxy       | ester          | 852               | 0.855            | 95          | 978      | 978      | 942      | 769        |
| 3-methyl-2(5H)-furanone                  | 22122-36-7 | 287215    | -              | Oxy       | ketone         | 854               | 1.755            | 98          | 980      | 979      | 924      | 861        |
| 4-Ethyltoluene                           | 622-96-8 | 161892    | -              | HC        | monocyclic aromatic | 858               | 0.45             | 120         | 981      | 977      | 928      | 912        |
| beta-pinene                              | 18172-67-3 | 2555045   | -              | HC        | monoterpene    | 858               | 0.37             | 93          | 981      | 980      | 948      | 936        |

Continued on next page
| Tentative Identification | CAS    | Peak Area | Health Effects | Class      | Subclass     | $t_R^1$ (s) | $t_R^2$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|--------------------------|--------|-----------|----------------|------------|--------------|-------------|-------------|------------|----------|----------|----------|------------|
| Heptanenitrile           | 629-08-3 | 127966    | -              | Nit        | nitrile      | 858         | 1.065       | 82         | 981      | 985      | 890      | 777        |
| beta-terpinene           | 99-84-3  | 326085    | -              | HC         | monoterpene  | 860         | 0.26        | 93         | 982      | 988      | 889      | 850        |
| Phenol                   | 108-95-2 | 23963163  | G3             | Oxy        | alcohol      | 862         | 0.5         | 94         | 983      | 984      | 968      | 964        |
| alpha-Methylstyrene      | 98-83-9  | 228795    | G2B            | HC         | monomeric    | 866         | 0.46        | 118        | 985      | 986      | 942      | 914        |
| 5-Hepten-2-one, 6-methyl- | 110-93-0 | 1141547   | -              | Oxy        | ketone       | 868         | 0.77        | 43         | 986      | 985      | 949      | 935        |
| Benzonitrile             | 100-47-0 | 6747487   | M              | Nit        | nitrile      | 874         | 1.01        | 103        | 989      | 989      | 941      | 941        |
| beta-Myrcene             | 123-35-3 | 5721453   | G2B            | HC         | monoterpene  | 878         | 0.355       | 69         | 990      | 986      | 957      | 950        |
| 2-Octanone               | 111-13-7 | 176549    | -              | Oxy        | ketone       | 880         | 0.795       | 58         | 991      | 990      | 898      | 815        |
| Cyclohexanone, 4-methylidene- | 29648-66-6 | 160763   | -              | Oxy        | ketone       | 880         | 1.1         | 82         | 991      | NA       | 813      | 754        |
| 1-Decene                 | 872-05-9  | 452605    | -              | HC         | alkene       | 882         | 0.325       | 56         | 992      | 992      | 913      | 908        |
| trans,trans-2,8-decadiene | 19398-85-7 | 164847   | -              | HC         | alkene       | 882         | 0.44        | 67         | 992      | 998      | 753      | 692        |
| 3-Methylstyrene          | 100-80-1  | 115001    | G3             | HC         | monocyclic   | 884         | 0.445       | 117        | 993      | 991      | 856      | 798        |
| 2-Furanmethanol, acetate | 623-17-6  | 323533    | M              | Oxy        | ester        | 884         | 0.68        | 81         | 993      | 995      | 950      | 936        |
| 3,3-dimethyl-6-methylenecyclohexene | 20185-16-4 | 393782    | -              | HC         | monocyclic   | 884         | 0.43        | 107        | 993      | 997      | 856      | 855        |
| 1H-Pyrrole, 1-butyl-     | 589-33-3  | 166688    | -              | Het        | pyrrole      | 888         | 0.585       | 80         | 995      | NA       | 913      | 897        |
| 1,2-Propadienylbenzene   | 2327-99-3 | 53815     | -              | HC         | monocyclic   | 888         | 0.475       | 116        | 995      | NA       | 895      | 801        |
| 2-Cyclopenten-1-one, 3,4-dimethyl- | 30434-64-1 | 196277   | -              | Oxy        | ketone       | 888         | 1.21        | 95         | 995      | 986      | 901      | 837        |
| 4-methylstyrene          | NA      | 806934    | -              | HC         | monocyclic   | 894         | 0.49        | 118        | 997      | 995      | 911      | 871        |
| Pyrazine, 2-ethyl-6-methyl- | 13925-03-6 | 495075    | -              | Het        | pyrazine     | 896         | 0.54        | 121        | 998      | 998      | 923      | 918        |
| Benzofuran               | 2792-39-4 | 443879    | G2B            | Het        | furan        | 898         | 0.555       | 90         | 999      | 1000     | 957      | 940        |

Continued on next page
| Tentative Identification                        | CAS      | Peak Area | Health Effects | Class | Subclass | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI<sup>*</sup> | Lib. RI<sup>*</sup> | Reverse<sup>†</sup> | Similarity<sup>‡</sup> |
|------------------------------------------------|----------|-----------|----------------|-------|----------|-----------|-----------|------------|---------------------|---------------------|---------------------|---------------------|
| 2,6-Octadiene, 2,6-dimethyl-                  | 2792-39-4| 1081849   | -              | HC    | alkene   | 898       | 0.31      | 69         | 999                 | 990                 | 919                 | 919                 |
| Decane                                         | 124-18-5 | 347655    | X              | HC    | alkane   | 902       | 0.305     | 57         | 1001                | 1000                | 942                 | 932                 |
| Pyrazine, trimethyl-                           | 14667-55-1| 1826615   | -              | Het   | pyrazine | 906       | 0.495     | 42         | 1003                | 1003                | 914                 | 914                 |
| Pyrazine, 2-ethyl-3-methyl-                    | 15707-23-0| 237534    | -              | Het   | pyrazine | 906       | 0.505     | 121        | 1003                | 1003                | 852                 | 841                 |
| Dehydroxylinalool oxide                       | 54750-69-5| 135697    | -              | Het   | furan    | 914       | 0.45      | 67         | 1007                | 1007                | 889                 | 863                 |
| alpha-Phellandrene                             | 99-83-2  | 1494367   | -              | HC    | monoterpe | 918       | 0.36      | 93         | 1009                | 1009                | 923                 | 919                 |
| Isobutylbenzene                                | 538-93-2 | 32384     | -              | HC    | aromatic | 920       | 0.425     | 134        | 1010                | 1009                | 966                 | 917                 |
| 1-Pyrrolidinylacetonitrile                     | 29134-29-0| 96879     | X              | Het   | pyridine | 922       | 0.925     | 82         | 1011                | NA                  | 902                 | 839                 |
| (-)-3-carene                                   | 20296-50-8| 1115470   | -              | HC    | monoterpe | 924       | 0.35      | 93         | 1012                | 1010                | 932                 | 929                 |
| Oxalic acid, allyl octyl ester                 | NA       | 200293    | -              | Oxy   | ester    | 930       | 0.33      | 57         | 1015                | NA                  | 872                 | 850                 |
| 3-Pyridinecarbonitrile                         | 100-54-9 | 477481    | X              | Het   | pyridine | 930       | 1.115     | 104        | 1015                | 1012                | 940                 | 839                 |
| 7-vinylbicyclo[4.2.0]oct-1-ene                 | NA       | 144355    | -              | HC    | alicyclic | 938       | 0.38      | 91         | 1019                | 1023                | 779                 | 760                 |
| gamma-Terpinene                                | 99-85-4  | 1085572   | M              | HC    | monoterpe | 940       | 0.36      | 93         | 1020                | 1023                | 913                 | 910                 |
| 2,6-dimethylnonane                             | 17302-28-2| 53493     | -              | HC    | alkane   | 946       | 0.32      | 71         | 1023                | 1024                | 897                 | 790                 |
| Benzoazole                                     | 273-53-0 | 27508     | -              | Nit   | oxazole  | 946       | 0.615     | 64         | 1023                | NA                  | 901                 | 790                 |
| Benzene, (2-methyl-2-propenyl)-                | 3290-53-7| 135613    | -              | HC    | monocyclic | 948       | 0.415     | 117        | 1024                | 1022                | 894                 | 824                 |
| p-Methylanisole                                | 104-93-8 | 185341    | X              | Oxy   | ether    | 948       | 0.52      | 122        | 1024                | 1024                | 938                 | 916                 |
| Benzene, 1,2,3-trimethyl-                      | 526-73-8 | 881976    | M              | HC    | monocyclic | 950       | 0.47      | 105        | 1025                | 1028                | 939                 | 929                 |
| Mesitylene                                     | 108-67-8 | 881976    | M              | HC    | monocyclic | 950       | 0.47      | 105        | 1025                | 1013                | 941                 | 933                 |
| 4,4-Dimethyl-2-cyclopenten-1-one               | 22748-16-9| 82207     | -              | Oxy   | ketone   | 950       | 1.35      | 95         | 1025                | NA                  | 904                 | 793                 |

Continued on next page
| Tentative Identification | CAS     | Peak Area | Health Effects | Class | Subclass | \( t_R \) (s) | \( 2 t_R \) (s) | Quant Mass | Exp. RI | Lib. RI | Reverse \(^1\) | Similarity \(^1\) |
|-------------------------|---------|----------|----------------|-------|----------|-------------|-------------|------------|--------|--------|--------------|------------|
| 4-butylcyclohexene      | 21524-26-5 | 131289   | -              | HC    | alicyclic | 954         | 0.365       | 54         | 1026   | 1036   | 769          | 753        |
| Bicyclo[4.2.0]oct-1-ene, 7-endo-ethenyl- | NA | 40281     | -              | HC    | alicyclic | 956         | 0.385       | 106        | 1027   | NA     | 830          | 816        |
| α-Cymene                | 527-84-4  | 3399473  | -              | HC    | monocyclic aromatic | 956         | 0.4         | 119        | 1027   | 1027   | 963          | 952        |
| (±)-Carvomenthene       | 1195-31-9 | 393503   | -              | HC    | monoterpenes | 956         | 0.345       | 95         | 1027   | 1028   | 897          | 893        |
| 2-hydroxy-3-methyl-2-cyclopenten-1-one | 80-71-7  | 809831   | M              | Oxy   | ketone    | 962         | 0.835       | 112        | 1031   | 1028   | 929          | 918        |
| Indane                  | 496-11-7  | 1503230  | -              | HC    | alicyclic | 962         | 0.49        | 117        | 1030   | 1030   | 921          | 920        |
| D-Limonene              | 5989-27-5 | 8749710  | G3             | HC    | monoterpenes | 966         | 0.35        | 68         | 1032   | 1031   | 945          | 944        |
| beta-phellandrene       | 555-10-2  | 3257485  | -              | HC    | monoterpenes | 970         | 0.385       | 93         | 1034   | 1033   | 930          | 930        |
| Eucalyptol              | 470-82-6  | 1353566  | T              | Oxy   | alcohol   | 974         | 0.415       | 43         | 1036   | 1035   | 934          | 925        |
| 2-Acetylpyridine        | 1122-62-9 | 200388   | M              | Het   | pyridine  | 976         | 0.73        | 79         | 1037   | 1036   | 933          | 880        |
| alpha-oicimene          | 08/10/6874 | 507472  | -              | HC    | monoterpenes | 976         | 0.325       | 93         | 1037   | 1037   | 929          | 921        |
| Isocarvestene           | 1461-27-4 | 25815    | -              | HC    | monoterpenes | 986         | 0.34        | 93         | 1042   | 1032   | 805          | 731        |
| Benzene, 3-butenyl-     | 768-56-9  | 925404   | -              | HC    | monoterpenes | 994         | 0.425       | 91         | 1046   | 1038   | 954          | 948        |
| trans-beta-Ocimene      | 13877-91-3 | 2665767 | -              | HC    | monoterpenes | 998         | 0.345       | 93         | 1048   | 1046   | 948          | 947        |
| Indene                  | 95-13-6   | 2444987  | -              | HC    | polycyclic aromatic | 1000        | 0.515       | 116        | 1049   | 1049   | 935          | 935        |
| 1,2-Diethylbenzene      | 135-01-3  | 74047    | M              | HC    | monoterpenes | 1002        | 0.41        | 119        | 1050   | 1048   | 835          | 791        |
| Benzene, 1-methyl-3-propyl- | 1074-43-7 | 402885  | -              | HC    | monoterpenes | 1010        | 0.415       | 105        | 1054   | 1055   | 908          | 895        |
| Tentative Identification                          | CAS      | Peak Area | Health Effects | Class   | Subclass          | 1<sub>t<sub>R</sub>(s) | 2<sub>t<sub>R</sub>(s) | Quant Mass | Exp. RI† | Lib. RI‡ | Reverse† | Similarity‡ |
|-------------------------------------------------|----------|-----------|----------------|---------|-------------------|-------------------------|-------------------------|-------------|----------|----------|----------|-------------|
| 1-(2-methylbutyl)-Pyrrole                        | 13678-55-2 | 510794    |                | Het     | pyrrole           | 1012                    | 0.555                   | 81          | 1055     | NA       | 905      | 783         |
| Benzene, 1-methyl-2-(2-propenyl)-               | 1587-04-8 | 71954     |                | HC      | monocyclic aromatic | HC                     | 1016                    | 0.435                   | 117         | 1057     | 1055     | 881      | 807         |
| o-Cresol                                        | 95-48-7  | 3029911   |                | G3      | Oxy alcohol       | 1018                    | 0.49                    | 108         | 1058     | 1058     | 944      | 943         |
| Benzene, 1-methyl-4-propyl                      | 1074-55-1 | 311167    |                | HC      | monocyclic aromatic | HC                     | 1020                    | 0.405                   | 105        | 1059     | 1059     | 889      | 872         |
| 3,5-dimethyl-1,2-cyclopentadione (caramel dione) | 13494-07-0 | 70043     |                | Oxy     | ketone            | 1020                    | 0.76                    | 126         | 1059     | 1048     | 835      | 793         |
| Benzene, 1,4-diethyl                            | 105-05-5 | 323348    |                | HC      | monocyclic aromatic | HC                     | 1022                    | 0.405                   | 119         | 1059     | 1057     | 908      | 901         |
| Butylbenzene                                    | 104-51-8 | 508729    |                | HC      | monocyclic aromatic | HC                     | 1022                    | 0.425                   | 92          | 1059     | 1058     | 910      | 895         |
| Phenyl acetate                                  | 122-79-2 | 459552    |                | Oxy     | ester             | 1024                    | 0.83                    | 94          | 1061     | 1065     | 944      | 917         |
| alpha-terpinene                                 | 99-86-5  | 144721    |                | M       | monoterpenes      | 1026                    | 0.33                    | 107         | 1061     | 1058     | 904      | 879         |
| 2-Cyclopenten-1-one, 2,3,4-trimethyl-            | 28790-86-5 | 94737     |                | Oxy     | ketone            | 1026                    | 0.935                   | 109         | 1062     | 1058     | 902      | 817         |
| Benzene, 1-propynyl-                            | 673-32-5 | 125307    |                | HC      | monocyclic aromatic | HC                     | 1034                    | 0.46                    | 115         | 1065     | 1058     | 909      | 811         |
| 2-Amino-4-methylpyrimidine                      | 108-52-1 | 260315    |                | Het     | pyrimidine        | 1036                    | 0.575                   | 109         | 1066     | NA       | 846      | 766         |
| Benzene, 1-methyl-2-propyl                      | 1074-17-5 | 335361    |                | HC      | monocyclic aromatic | HC                     | 1040                    | 0.435                   | 105        | 1068     | 1065     | 898      | 885         |
| Benzene, isobutenyl-                            | 768-49-0 | 122986    |                | HC      | monocyclic aromatic | HC                     | 1044                    | 0.4         | 117        | 1070     | 1071     | 885       | 855       |
| 2-Acetylpyrrole                                 | 1072-83-9 | 736197    | M              | Het     | pyrrole           | 1046                    | 0.78                    | 94          | 1071     | 1072     | 933      | 880         |

Continued on next page
| Tentative Identification | CAS     | Peak Area  | Health Effects | Class    | Subclass | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse†  | Similarity‡ |
|--------------------------|---------|------------|----------------|----------|----------|----------|-----------|-----------|----------|----------|-----------|-------------|
| Acetophenone             | 98-86-2 | 720372     | M              | Oxy      | ketone   | 1046     | 0.845     | 105       | 1071     | 1071     | 958       | 952         |
| 2-Pyridinecarbonitrile   | 100-70-9| 777742     | -              | Het      | pyridine | 1046     | 1.36      | 104       | 1072     | 1069     | 968       | 901         |
| 4-thujanol               | 15826-82-1| 509930    | -              | Oxy      | alcohol  | 1050     | 0.51      | 71        | 1073     | 1073     | 940       | 916         |
| Benzenamine, 2-methyl-    | 636-21-5| 51625      | M              | Nit      | amine    | 1054     | 0.62      | 106       | 1075     | 1072     | 920       | 787         |
| 5-Undecene, 4-methyl-    | NA      | 171241     | -              | HC       | alkene   | 1054     | 0.325     | 69        | 1075     | NA       | 836       | 804         |
| 2-Pyrrolidinone          | 616-45-5| 2747459    | M              | Het      | pyrrole  | 1060     | 1.465     | 85        | 1078     | 1078     | 949       | 913         |
| Pyrazine, 3-ethyl-2,5-dimethyl- | 13360-65-1 | 116804  | -              | Het      | pyrazine | 1060     | 0.465     | 136       | 1078     | 1078     | 916       | 807         |
| Benzene, 2-ethyl-1,4-dimethyl- | 1758-88-9 | 151788   | -              | HC       | aromatic | 1060     | 0.415     | 119       | 1078     | 1077     | 860       | 841         |
| m-Cresol                | 108-39-4| 10111666   | G3             | Oxy      | alcohol  | 1062     | 0.495     | 108       | 1079     | 1079     | 948       | 941         |
| 3-ethyl-2-cyclopenten-1-one | 5682-69-9 | 201452   | -              | Oxy      | ketone   | 1062     | 1.235     | 81        | 1079     | 1071     | 894       | 827         |
| Benzene, 4-ethyl-1,2-dimethyl- | 934-80-5 | 396644   | -              | HC       | aromatic | 1066     | 0.41      | 119       | 1081     | 1079     | 902       | 896         |
| Octanenitrile           | 124-12-9| 111024     | -              | Nit      | nitrile  | 1068     | 0.97      | 82        | 1082     | 1082     | 891       | 815         |
| 3-Methylbenzaldehyde     | 620-23-5| 71266      | -              | Oxy      | aldehyde | 1070     | 0.55      | 120       | 1083     | 1081     | 852       | 710         |
| 1,10-Undecadiene        | 13688-67-0| 115658   | -              | HC       | alkene   | 1072     | 0.33      | 67        | 1084     | 1083     | 936       | 855         |
| p-cymenene              | 1195-32-0| 382162     | -              | HC       | monoterpane | 1074     | 0.43      | 117       | 1085     | 1085     | 934       | 917         |
| Z-1,8-Dodecadiene       | NA      | 413966     | -              | HC       | alkene   | 1078     | 0.315     | 67        | 1087     | NA       | 882       | 795         |
| Benzene, 3-ethyl-1,2-dimethyl- | 933-98-2 | 276928   | -              | HC       | aromatic | 1078     | 0.4       | 119       | 1087     | 1088     | 904       | 892         |
| Linalyl oxide           | 5989-33-3| 189676     | -              | Het      | furan    | 1082     | 0.55      | 59        | 1089     | 1088     | 901       | 875         |
| Terpinolene (delta-terpinene) | 586-62-9 | 2818988 | -              | HC       | monoterpane | 1082     | 0.335     | 43        | 1089     | 1089     | 924       | 922         |
| 1H-Indene, 2,3-dihydromethyl- | 27133-93-3 | 56842   | -              | HC       | polycyclic | 1082     | 0.44      | 132       | 1089     | 1085     | 897       | 866         |
| Guaiacol                | 90-05-1 | 2679865    | X              | Oxy      | alcohol  | 1084     | 0.675     | 109       | 1090     | 1090     | 973       | 956         |

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Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke (Continued)

| Tentative Identification | CAS      | Peak Area | Health Effects | Class | Subclass               | 1<sub>tR</sub> (s) | 2<sub>tR</sub> (s) | Quant Mass | Exp. RI<sup>†</sup> | Lib. RI<sup>‡</sup> | Reverse<sup>†</sup> | Similarity<sup>‡</sup> |
|--------------------------|----------|-----------|----------------|-------|------------------------|-------------------|---------------|------------|----------------|----------------|----------------|----------------|
| 2-Nonanone               | 821-55-6 | 128119    | -              | Oxy   | ketone                 | 1086             | 0.72          | 58          | 1091           | 1091           | 925            | 767            |
| 1-Undecene               | 821-95-4 | 801561    | -              | HC    | alkene                 | 1088             | 0.295         | 56          | 1091           | 1091           | 937            | 935            |
| Benzene, 2-ethyl-1,3-dimethyl- | 04/04/2870 | 74533    | -              | HC    | monocyclic aromatic HC | 1088             | 0.425         | 119         | 1092           | 1087           | 859            | 806            |
| alpha-Naginatene         | 15186-51-3 | 39058    | -              | Het   | furan                  | 1090             | 0.39          | 150         | 1092           | 1093           | 841            | 797            |
| 3-Methylene-1,5,5-trimethylcyclohexene | 16609-28-2 | 57007    | -              | HC    | alicyclic HC           | 1090             | 0.33          | 121         | 1092           | NA             | 883            | 825            |
| m-cymenene               | 1124-20-5 | 3205300   | -              | HC    | monocyclic aromatic HC | 1090             | 0.43          | 91          | 1092           | 1092           | 950            | 919            |
| (+)-Fenchone              | 1195-79-5 | 995577    | -              | Oxy   | ketone                 | 1090             | 0.76          | 81          | 1093           | 1088           | 937            | 935            |
| 3-Methylbenzonitrile      | 620-22-4 | 930665    | -              | Nit   | nitrile                | 1094             | 0.985         | 117         | 1095           | 1094           | 945            | 936            |
| Benzene, 1-ethenyl-4-ethyl- | 07/07/3454 | 176971   | -              | HC    | monocyclic aromatic HC | 1098             | 0.45          | 117         | 1096           | NA             | 894            | 864            |
| Benzoic acid, methyl ester | 93-58-3  | 291583    | -              | Oxy   | ester                  | 1102             | 0.66          | 105         | 1098           | 1098           | 929            | 880            |
| 4,4-dimethylcyclohexenone | 1073-13-8 | 45153     | -              | Oxy   | ketone                 | 1104             | 0.955         | 124         | 1100           | 1101           | 808            | 692            |
| Linalool                  | 78-70-6  | 7227942   | M              | Oxy   | alcohol                | 1106             | 0.43          | 71          | 1100           | 1101           | 953            | 953            |
| Undecane                  | 1120-21-4 | 906616   | X              | HC    | alkane                 | 1106             | 0.29          | 57          | 1100           | 1100           | 947            | 935            |
| sec-Pentylbenzene         | 2719-52-0 | 143311    | -              | HC    | monocyclic aromatic HC | 1110             | 0.39          | 105         | 1102           | 1098           | 844            | 802            |
| 2,5-dimethylstyrone       | 2039-89-6 | 204202    | -              | HC    | monocyclic aromatic HC | 1112             | 0.44          | 117         | 1103           | 1101           | 874            | 835            |
| 2-Undecene, (E)-          | 693-61-8  | 62499     | -              | HC    | alkene                 | 1114             | 0.29          | 70          | 1104           | 1104           | 870            | 858            |
| beta-terpineol            | 7299-41-4 | 622740    | -              | Oxy   | alcohol                | 1114             | 0.55          | 43          | 1105           | 1101           | 917            | 903            |
| Benzo furan, 2-methyl-     | 4265-25-2 | 606545    | -              | Het   | furan                  | 1122             | 0.54          | 131         | 1109           | 1108           | 919            | 903            |
| 6,7-dihydro-5H-Cyclopenta pyrazine | NA       | 320737    | -              | Het   | pyrazine               | 1126             | 0.6           | 119         | 1111           | 1104           | 955            | 869            |

Continued on next page
| Tentative Identification | CAS      | Peak Area | Health Effects | Class      | Subclass     | $1_R$ (s) | $2_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|--------------------------|----------|-----------|----------------|------------|--------------|-----------|-----------|------------|---------|---------|---------|------------|
| Phenol, 2,6-dimethyl-    | 576-26-1 | 460482    | X              | Oxy alcohol | HC monoterpene | 1126      | 0.51      | 107        | 1111    | 1111    | 949     | 933        |
| 2,3-Cyclopentenopyridine | 533-37-9 | 584415    | -              | Het pyridine | HC monoterpene | 1136      | 0.58      | 118        | 1116    | NA      | 896     | 892        |
| 1,3,8-Menthatriene       | 18368-95-1 | 540607   | -              | HC monoterpenes | 1136      | 0.38      | 91         | 1116    | 1118    | 913     | 895        |
| Benzene, 1-ethyl-4-methoxy- | 1515-95-3 | 66875    | -              | Oxy ether | HC monocyclic aromatic | 1136      | 0.48      | 121        | 1116    | 1110    | 919     | 893        |
| Phenylethyl Alcohol      | 60-12-8  | 135274    | X              | Oxy alcohol | HC monocyclic aromatic | 1142      | 0.59      | 92         | 1120    | 1119    | 905     | 814        |
| Benzoazoxole, 2-methyl- | 95-21-6  | 90966     | -              | Nit oxazole | HC alicyclic | 1144      | 0.57      | 133        | NA      | 1121    | 913     | 825        |
| 2-Cyclopenten-1-one, 3-ethyl-2-hydroxy- | 21835-01-8 | 159603 | -              | Oxy ketone | HC monocyclic aromatic | 1144      | 0.775     | 83         | 1121    | 1121    | 934     | 876        |
| Fenchol, exo-            | 22627-95-8 | 4705295 | -              | Oxy alcohol | HC monocyclic aromatic | 1150      | 0.48      | 81         | 1124    | 1120    | 958     | 954        |
| Benzene, 1,2,3,5-tetramethyl | 527-53-7  | 151631    | X              | HC monoterpene | 1150      | 0.415     | 119        | 1124    | 1123    | 785     | 772        |
| o-Cymenene               | 7399-49-7 | 129571    | -              | HC monoterpenes | 1152      | 0.455     | 117        | 1125    | 1117    | 890     | 842        |
| (E)-cyclodecene          | 2198-20-1 | 127075    | -              | HC alicyclic | 1154      | 0.34      | 54         | 1126    | 1122    | 846     | 798        |
| Benzene, 1-butenyl-, (E)- | 1005-64-7 | 587104    | -              | HC monocyclic aromatic | 1160      | 0.45      | 117        | 1129    | 1120    | 911     | 900        |
| Alloocimene              | 3016-19-1 | 287176    | -              | HC monoterpenes | 1160      | 0.37      | 121        | 1129    | 1128    | 926     | 916        |
| 2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-, trans- | 29803-81-4 | 240659 | -              | Oxy alcohol | HC monoterpenes | 1160      | 0.49      | 43         | 1129    | 1130    | 828     | 814        |
| Benzyl methyl ketone     | 103-79-7  | 567846    | -              | Oxy ketone | HC monoterpenes | 1162      | 0.875     | 43         | 1130    | 1124    | 947     | 916        |
| 2,6,6-Triethylbicyclo[3.1.1]hept-2-ol | 98510-89-5 | 1625956 | -              | Oxy alcohol | HC monoterpenes | 1164      | 0.5       | 99         | 1131    | 1130    | 909     | 909        |
| 3-Pyridinol, 2-methyl-   | 1121-25-1 | 363820    | -              | Het pyridine | HC monoterpenes | 1168      | 0.53      | 109        | 1133    | NA      | 889     | 802        |
| Cosmene                  | 460-01-5  | 59488     | -              | HC monoterpenes | 1168      | 0.43      | 119        | 1133    | 1132    | 919     | 880        |
| 2,5-Pyrrolinedione, 1-ethyl- | 2314-78-5 | 87341    | -              | Het pyrrole | HC monoterpenes | 1170      | 1.345     | 56         | 1135    | NA      | 911     | 753        |

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Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke (Continued)

| Tentative Identification                     | CAS    | Peak Area | Health Effects | Class | Subclass          | \[t_R (s)\] | \[2t_R (s)\] | Quant Mass | Exp. RI | Lib. RI | Reverse\(^1\) | Similarity\(^2\) |
|----------------------------------------------|--------|-----------|----------------|-------|-------------------|-------------|-------------|------------|--------|--------|--------------|------------------|
| 1-Methyl-2-phenylcyclopropane                | NA     | 173563    | -              | HC    | alicyclic HC      | 1172        | 0.465       | 117        | 1135   | NA     | 873          | 854              |
| 3,4-Dimethylcumene                           | NA     | 353153    | -              | HC    | monocyclic aromatic HC | 1174        | 0.385       | 133        | 1136   | 1139   | 889          | 887              |
| p-Mentha-1,5,8-triene                        | 21195-59-5 | 629040  | -              | HC    | monoterpene       | 1180        | 0.4         | 91         | 1140   | 1139   | 923          | 922              |
| 2-Ethylphenol                                | 90-00-6 | 1173803   | X              | Oxy   | alcohol nitrile   | 1182        | 0.45        | 107        | 1141   | 1140   | 939          | 920              |
| Benzylic nitrile                             | 140-29-4 | 3474037  | M              | Nit   | nitrile          | 1184        | 0.985       | 90         | 1142   | 1142   | 938          | 935              |
| Cyclopentane, hexyl-                        | 4457-00-5 | 46920    | -              | HC    | alicyclic HC      | 1184        | 0.32        | 69         | 1142   | 1141   | 883          | 802              |
| 4-Methylindane                               | 824-22-6 | 406876    | -              | HC    | polycyclic aromatic HC | 1188        | 0.41        | 117        | 1144   | 1142   | 887          | 878              |
| N,N,O-Triacetylhydroxylamine                 | 17720-63-7 | 441976  | -              | Misc  | acetamide         | 1188        | 1.605       | 43         | 1145   | NA     | 931          | 812              |
| Ipsdienol                                    | 35628-00-3 | 392218  | -              | Oxy   | alcohol          | 1190        | 0.495       | 85         | 1145   | 1147   | 830          | 819              |
| 3-Methylheptyl acetate                       | 72218-58-7 | 104481  | -              | Oxy   | ester            | 1192        | 0.565       | 70         | 1146   | NA     | 953          | 869              |
| Epoxyterpinolene                             | NA     | 1934593   | -              | Oxy   | epoxide          | 1194        | 0.575       | 79         | 1147   | 1138   | 966          | 769              |
| o-Ethylbenzonitrile                          | 34136-59-9 | 69989   | -              | Nit   | nitrile          | 1198        | 0.845       | 116        | 1149   | NA     | 906          | 773              |
| Cis-2-pinanol                                | 4948-28-1 | 223166   | -              | Oxy   | alcohol          | 1204        | 0.535       | 99         | 1152   | 1143   | 889          | 888              |
| 5-Methylindane                               | 874-35-1 | 180401    | -              | HC    | alicyclic HC      | 1206        | 0.435       | 117        | 1153   | 1147   | 829          | 816              |
| 1,4-Dimethyl-4-acetylcyclohexene             | 43219-68-7 | 32841   | -              | Oxy   | ketone           | 1208        | 0.695       | 109        | 1155   | 1152   | 877          | 813              |
| Phenol, 2,4-dimethyl-2-Undecyne              | 105-67-9 | 81632    | -              | Oxy   | alcohol          | 1210        | 0.455       | 93         | 1156   | 1156   | 908          | 858              |
| 1-Methylindene                               | 767-59-9 | 436825    | -              | HC    | polycyclic aromatic HC | 1212        | 0.475       | 115        | 1157   | 1149   | 883          | 836              |
| 2,6-Dimethylbenzonitrile                     | 6575-13-9 | 61839    | -              | Nit   | nitrile          | 1212        | 0.815       | 116        | 1157   | NA     | 910          | 821              |

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Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke (Continued)

| Tentative Identification | CAS     | Peak Area | Health Effects | Class          | Subclass       | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|--------------------------|---------|-----------|----------------|----------------|----------------|-----------|------------|------------|---------|---------|---------|------------|
| 2,5-Pyrrolidinedione    | 123-56-8| 374850    |                | Het            | pyrrole        | 1214      | 1.235      | 99         | 1158    | NA      | 892    | 760        |
| 1H-Pyrrole-3-carbonitrile| 7126-38-7| 1070634   |                | Het            | pyrrole        | 1216      | 0.795      | 92         | 1159    | NA      | 877    | 821        |
| Glutarimide             | 1121-89-7| 4097543   |                | Nit            | imide          | 1216      | 1.27       | 42         | 1159    | 1154    | 884    | 882        |
| Phenol, 3,4-dimethyl-   | 95-65-8  | 175301    |                | Oxy            | alcohol        | 1216      | 0.475      | 107        | 1159    | 1155    | 875    | 787        |
| 4-Methoxystyrene        | 637-69-4 | 70954     |                | Oxy            | ether          | 1216      | 0.53       | 134        | 1159    | 1158    | 847    | 756        |
| Naphthalene, 1,4-dihydro-| 612-17-9| 840051    |                | HC             | alicyclic HC   | 1218      | 0.505      | 130        | 1160    | 1167    | 910    | 903        |
| Benzene, pentyl-        | 538-68-1 | 558678    |                | HC             | monocyclic HC  | 1218      | 0.4        | 92         | 1160    | 1160    | 941    | 932        |
| 5-Pentylcyclohexa-1,3-diene | 56318-84-4| 163521    |                | HC             | alicyclic HC   | 1222      | 0.35       | 79         | 1162    | 1161    | 860    | 821        |
| 2-Undecene, 9-methyl-, (Z)-p-Tolyl acetate | 74630-45-8 | 41504     |                | HC             | alkene        | 1224      | 0.31       | 70         | 1163    | NA      | 856    | 791        |
| Acetophenone, 2'-hydroxy-| 118-93-4| 125053    |                | Oxy            | ketone        | 1232      | 0.765      | 121        | 1167    | 1167    | 858    | 777        |
| Naphthalene, 1,2,3,4-tetrahydro- | 119-64-2| 129659    | X              | HC             | monocyclic aromatic HC | 1232 | 0.435      | 104        | 1167    | 1164    | 811    | 717        |
| p-Isobutyltoluene       | 06/04/5161| 275852    |                | HC             | monocyclic aromatic HC | 1234 | 0.42       | 105        | 1168    | NA      | 854    | 843        |
| 1H-Pyrrole-2,5-dione, 3,4-dimethyl- | 17825-86-4| 944293    |                | Het            | pyrrole        | 1236      | 1.035      | 125        | 1170    | NA      | 961    | 835        |
| Undecane, 3-methyl-     | 1002-43-3| 52333     |                | HC             | alkane        | 1238      | 0.305      | 57         | 1170    | 1170    | 911    | 782        |
| 4-Ethylphenol           | 123-07-9 | 3759309   |                | Oxy            | alcohol       | 1238      | 0.48       | 107        | 1171    | 1170    | 929    | 927        |
| 1-Propanone, 1-phenyl-  | 93-55-0  | 211300    | X              | Oxy            | ketone        | 1238      | 0.72       | 105        | 1171    | 1173    | 942    | 908        |
| Pyrrolidine, 1-acetyl-  | 4030-18-6| 160547    |                | Het            | pyrrole       | 1240      | 1.395      | 70         | 1172    | 1162    | 934    | 861        |
| Naphthalene, 1,2-dihydro-| 447-53-0| 301186    |                | HC             | alicyclic HC  | 1240      | 0.46       | 130        | 1172    | 1166    | 946    | 937        |
| (+)-Borneol             | 464-43-7 | 3907231   |                | Oxy            | alcohol       | 1252      | 0.51       | 95         | 1178    | 1177    | 926    | 926        |

Continued on next page
| Tentative Identification | CAS     | Peak Area | Health Effects | Class   | Subclass                     | \( t_R \) (s) | \( 2t_R \) (s) | Quant Mass | Exp. RI \(^\ast\) | Lib. RI \(^\ast\) | Reverse \(^\dagger\) | Similarity \(^\ddagger\) |
|-------------------------|---------|-----------|----------------|---------|------------------------------|--------------|--------------|------------|-----------------|-----------------|-----------------|-----------------|
| Benzonitrile, 3,5-dimethyl- | 22445-42-7 | 177588    | -              | Nit     | nitrile                      | 1256         | 0.865        | 116        | 1180            | NA              | 895             | 881             |
| 1H-Pyrrole, 1-(2-furanylmethyl)- | 1438-94-4 | 1683279   | -              | Het     | pyrrole                      | 1258         | 0.56         | 81         | 1181            | 1182            | 936             | 922             |
| Benzene, (1-methyl-1-butenyl)- | 53172-84-2 | 113835    | -              | HC      | monocyclic aromatic HC       | 1258         | 0.4          | 131        | 1181            | 1184            | 870             | 847             |
| Phenol, 2,3-dimethyl- | 526-75-0 | 363156    | -              | Oxy     | alcohol                      | 1258         | 0.485        | 107        | 1181            | 1180            | 909             | 873             |
| 1H-Pyrrolo[2,3-B]pyridine | 271-63-6 | 100746    | -              | Het     | pyridine                     | 1262         | 1.425        | 118        | 1184            | 1192            | 864             | 744             |
| 1,11-Dodecadiene | 5876-87-9 | 313414    | -              | HC      | alkene                       | 1262         | 0.315        | 55         | 1183            | 1179            | 926             | 888             |
| Limonen-4-ol | 01/02/3419 | 1980399   | -              | Oxy     | alcohol                      | 1262         | 0.45         | 69         | 1183            | 1181            | 903             | 855             |
| 4-Terpinol | 562-74-3 | 1590323   | -              | Oxy     | alcohol                      | 1266         | 0.46         | 71         | 1185            | 1186            | 910             | 908             |
| (3Z,5E)-1,3,5-Undecatriene | 19883-27-3 | 48622     | -              | HC      | alkene                       | 1268         | 0.38         | 80         | 1186            | 1187            | 923             | 835             |
| 2-Isopropylphenol | 88-69-7 | 215658    | -              | Oxy     | alcohol                      | 1270         | 0.475        | 121        | 1188            | 1184            | 888             | 834             |
| 5-Dodecene, (E)- | 7206-16-8 | 35095     | -              | HC      | alkene                       | 1272         | 0.305        | 55         | 1189            | 1182            | 884             | 811             |
| 1H-Indene, 1,3-dimethyl- | 2177-48-2 | 487632    | -              | HC      | alicylic HC                  | 1274         | 0.44         | 129        | 1190            | NA              | 907             | 889             |
| p-Cymen-8-ol | 1197-01-9 | 3200547   | -              | Oxy     | alcohol                      | 1276         | 0.49         | 135        | 1191            | 1190            | 947             | 943             |
| 1H-Indene, 2,3-dihydro-1,6-dimethyl- | 17059-48-2 | 427087    | -              | HC      | alicylic HC                  | 1278         | 0.39         | 131        | 1192            | NA              | 909             | 907             |
| 1-Dodecene | 112-41-4 | 763252    | -              | HC      | alkene                       | 1278         | 0.3         | 56         | 1192            | 1192            | 916             | 916             |
| Ethanone, 1-(3-methylphenyl)- | 585-74-0 | 374857    | -              | Oxy     | ketone                       | 1278         | 0.795        | 119        | 1192            | 1192            | 956             | 920             |
| Naphthalene | 91-20-3 | 3472044   | G2B            | HC      | polycyclic aromatic HC       | 1280         | 0.55         | 128        | 1193            | 1192            | 961             | 958             |
| Phenol, 2-methoxy-4-methyl- | 93-51-6 | 462417    | M              | Oxy     | alcohol                      | 1282         | 0.64         | 123        | 1194            | 1194            | 936             | 930             |
| 4-Dodecene | 2030-84-4 | 29606     | -              | HC      | alkene                       | 1284         | 0.295        | 56         | 1195            | 1187            | 881             | 830             |
| alpha-Terpinol | 98-55-5 | 9365585   | -              | Oxy     | alcohol                      | 1292         | 0.475        | 59         | 1199            | 1198            | 953             | 943             |
| 1H-Indene, 2,3-dihydro-1,3-dimethyl- | 4175-53-5 | 83583     | -              | HC      | alicylic HC                  | 1294         | 0.42         | 131        | 1200            | NA              | 825             | 784             |

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Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke (Continued)

| Tentative Identification | CAS      | Peak Area | Health Effects | Class    | Subclass | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|--------------------------|----------|-----------|----------------|----------|----------|----------|-----------|------------|----------|----------|----------|--------------|
| Dodecane                | 112-40-3 | 1171663   | -              | HC       | alkane   | 1294     | 0.295     | 57         | 1200     | 1200     | 942      | 940          |
| Phenol, 3-ethyl-         | 620-17-7 | 26143     | -              | Oxy      | alcohol  | 1294     | 0.515     | 133        | 1200     | 1195     | 859      | 791          |
| Ethyl-2-benzofuran      | 3131-63-3| 249985    | -              | Het      | furan    | 1300     | 0.5       | 131        | 1204     | 1207     | 875      | 787          |
| m-Ethylbenzonitrile     | 34136-57-7| 100480    | -              | Nit      | nitrile  | 1304     | 0.935     | 116        | 1206     | Na       | 912      | 766          |
| Phenol, 2,4,6-trimethyl- | 527-60-6 | 185633    | M              | Oxy      | alcohol  | 1310     | 0.475     | 121        | 1210     | 1211     | 944      | 895          |
| alpha-Phellandrene epoxide | 72138-69-3| 57317    | -              | Oxy      | epoxide  | 1310     | 0.5       | 92         | 1210     | 1211     | 817      | 758          |
| Undecane, 2,6-dimethyl- | 17301-23-4| 1051696   | -              | HC       | alkane   | 1316     | 0.305     | 57         | 1213     | 1213     | 953      | 942          |
| 3-Carvomenthenol         | 16721-39-4| 358871    | -              | Oxy      | alcohol  | 1318     | 0.49      | 84         | 1214     | 1214     | 865      | 810          |
| Benzoic acid, 4,7-dimethyl- | 28715-26-6| 529888   | -              | Het      | furan    | 1332     | 0.5       | 145        | 1222     | 1220     | 876      | 868          |
| 2,3-Dihydrobenzoic acid | 496-16-2 | 9360544   | -              | Het      | furan    | 1336     | 0.48      | 120        | 1224     | 1224     | 911      | 897          |
| 2,3-Dimethylbenzoic acid | 3782-00-1| 103816    | -              | Het      | furan    | 1340     | 0.515     | 131        | 1227     | NA       | 851      | 752          |
| trans-Chrysanthene acetate | 54324-99-1| 745903   | -              | Oxy      | ester    | 1342     | 0.445     | 43         | 1228     | NA       | 731      | 725          |
| Furan, 3-phenyl-         | 13679-41-9| 139070    | -              | Het      | furan    | 1344     | 0.53      | 115        | 1229     | 1228     | 923      | 848          |
| Phenol, 2-ethyl-6-methyl- | 1687-64-5| 599337    | -              | Oxy      | alcohol  | 1346     | 0.44      | 121        | 1230     | 1236     | 910      | 834          |
| 1H-Pyrrole, 2,5-dione, 3-ethyl-4-methyl- | 20189-42-8| 259561   | -              | Het      | pyrrole  | 1358     | 0.95      | 139        | 1237     | 1238     | 914      | 891          |
| Phenol, 4-ethyl-3-methyl- | 1123-94-0| 1026040   | -              | Oxy      | alcohol  | 1364     | 0.45      | 121        | 1241     | 1239     | 920      | 891          |
| Benzenepropanonitrile   | 645-59-0 | 3554324   | -              | Nit      | nitrile  | 1368     | 1.01      | 91         | 1243     | 1243     | 950      | 941          |
| Cyclohexane, hexyl-     | 4292-75-5 | 26323     | -              | HC       | alicyclic HC | 1370     | 0.32      | 82         | 1244     | 1244     | 904      | 780          |
| 1H-Indene, 2,3-dimethyl- | 4773-82-4| 66291     | -              | HC       | aromatic polycyclic HC | 1370     | 0.445     | 129        | 1244     | NA       | 864      | 780          |
| 2-Butanone, 4-phenyl-    | 2550-26-7 | 78349     | -              | Oxy      | ketone   | 1376     | 0.79      | 105        | 1248     | 1251     | 898      | 849          |
| Isoquinoline            | 119-65-3 | 245664    | M              | Nit      | aza-arene polycyclic aromatic HC | 1378     | 0.64      | 129        | 1249     | 1255     | 945      | 918          |
| 2-Ethyl-1-H-indene      | 17059-50-6| 151437    | -              | HC       | aromatic polycyclic HC | 1382     | 0.45      | 129        | 1251     | NA       | 900      | 838          |
| Tentative Identification                          | CAS    | Peak Area | Health Effects | Class    | Subclass   | $t_R$ (s) $^1$ | $t_R$ (s) $^2$ | Quant Mass | Exp. RI $^*$ | Lib. RI $^*$ | Reverse $^1$ | Similarity $^1$ |
|------------------------------------------------|--------|-----------|----------------|----------|------------|---------------|---------------|------------|--------------|--------------|-------------|----------------|
| Hexanoic acid, 2-methylbutyl ester            | 2601-13-0 | 183766   | -              | Oxy ester |            | 1382          | 0.505         | 99         | 1251         | 1251         | 930          | 915            |
| Geraniol                                       | 106-25-2  | 1386581  | -              | Oxy alcohol | monocyclic aromatic HC | 1386          | 0.465         | 69         | 1253         | 1253         | 936          | 905            |
| Benzene, (1,3-dimethylbutyl)-                 | 19219-84-2 | 116244   | -              | HC        |            | 1388          | 0.37          | 105        | 1254         | NA           | 828          | 778            |
| Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-      | 32367-54-7 | 51651    | -              | HC        | polycyclic aromatic HC | 1390          | 0.395         | 104        | 1255         | NA           | 839          | 799            |
| Naphthalene, 1,2-dihydro-3-methyl-            | 2717-44-4  | 98985    | -              | HC        | polycyclic aromatic HC | 1394          | 0.445         | 129        | 1258         | NA           | 823          | 762            |
| Phenol, 4-propyl-                             | 645-56-7   | 366802   | -              | Oxy alcohol | monocyclic aromatic HC | 1402          | 0.465         | 107        | 1262         | 1262         | 869          | 831            |
| Benzene, hexyl-                               | 1077-16-3  | 246007   | -              | HC        | polycyclic aromatic HC | 1404          | 0.38          | 92          | 1263         | 1263         | 871          | 865            |
| Picolinamide                                  | 1452-77-3  | 643635   | -              | Het pyridine |            | 1410          | 0.955         | 79          | 1267         | 1268         | 948          | 883            |
| Quinoline, 5,6,7,8-tetrahydro-1-(5-methylfurfuryl)-Pyrrrole | 13678-52-9  | 392724   | -              | Het pyrrrole |            | 1424          | 0.5          | 95          | 1275         | NA           | 938          | 773            |
| 1H-Indole, 1-methyl-                           | 603-76-9   | 66277    | -              | Nit aza-arene |            | 1424          | 0.695         | 131        | 1275         | 1273         | 865          | 779            |
| Phenol, 2,3,5-trimethyl-                       | 697-82-5   | 117015   | -              | Oxy alcohol |            | 1426          | 0.475         | 121        | 1276         | 1276         | 864          | 721            |
| 1,4-Benzenedicarbonitrile                     | 623-26-7   | 323451   | -              | Nit nitrile |            | 1430          | 1.495         | 128        | 1279         | NA           | 945          | 793            |
| Phenol, 4-ethyl-2-methoxy-                    | 2785-89-9  | 183169   | -              | Oxy alcohol |            | 1430          | 0.61          | 137        | 1279         | 1278         | 917          | 886            |
| 5H-Benzocycloheptene, 6,7-dihydro-            | 7125-62-4  | 89144    | -              | HC alicyclic HC |            | 1432          | 0.435         | 129        | 1280         | 1269         | 858          | 814            |
| 1,12-Tridecadiene                             | 21964-48-7  | 301849   | -              | HC alkene |            | 1440          | 0.315         | 55          | 1284         | 1279         | 909          | 865            |
| 1H-Pyrrole, 1-phenyl-                          | 635-90-5   | 50635    | -              | Het pyrrrole |            | 1442          | 0.53          | 143        | 1285         | NA           | 865          | 774            |
| 1,2,3-Trimethylindene                          | 4773-83-5  | 167351   | -              | HC alicyclic HC |            | 1444          | 0.42          | 143        | 1286         | NA           | 866          | 858            |
| Bornyl acetate                                | 76-49-3    | 279818   | -              | Oxy ester |            | 1448          | 0.615         | 95          | 1289         | 1289         | 933          | 928            |
| Phenol, 2-ethenyl-, acetate                   | 63600-35-1 | 176968   | -              | Oxy ester |            | 1448          | 0.76          | 120        | 1289         | NA           | 916          | 810            |

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| Tentative Identification | CAS    | Peak Area | Health Effects | Class       | Subclass            | $t_R$ (s) | Mass (g/mol) | Quant. Mass | Exp. RI $^*$ | Lib. RI $^*$ | Reverse $^+$ | Similarity $^+$ |
|--------------------------|--------|-----------|----------------|-------------|---------------------|-----------|--------------|-------------|--------------|--------------|---------------|----------------|
| 1H-Inden-1-one, 2,3-dihydro- | 83-33-0 | 364862    | -              | Oxy         | ketone              | 1448      | 0.845        | 104         | 1289         | 1285         | 943           | 857            |
| 1H-Indene, 1-ethylidene- | 2471-83-2 | 51136    | -              | HC          | polycyclic aromatic | 1450      | 0.545        | 141         | 1290         | NA           | 913           | 767            |
| 2-Tridecene, (Z)-        | 41446-58-6 | 1079417  | -              | HC          | alkene              | 1454      | 0.305        | 56          | 1292         | 1296         | 932           | 920            |
| Thymol                   | 89-83-8  | 25723     | -              | Oxy         | alcohol             | 1456      | 0.42         | 135         | 1293         | 1293         | 935           | 770            |
| Carvacrol                | 499-75-2 | 131905    | X              | Oxy         | alcohol             | 1460      | 0.45         | 135         | 1296         | 1296         | 901           | 852            |
| Indole                   | 120-72-9 | 9507460   | -              | Nit         | aza-arenne          | 1466      | 0.655        | 90          | 1299         | 1299         | 936           | 925            |
| Tridecane                | 629-50-5 | 1134358   | -              | HC          | alkane              | 1468      | 0.29         | 57          | 1300         | 1300         | 959           | 947            |
| (1-Methylbuta-1,3-dietyl) | 54758-36-0 | 128719   | -              | HC          | monocyclic aromatic | 1468      | 0.465        | 129         | 1300         | NA           | 857           | 811            |
| 2-Ethyl-4,5-dimethylphenol | 2219-78-5 | 132802   | -              | Oxy         | alcohol             | 1472      | 0.44         | 135         | 1303         | 1305         | 873           | 799            |
| 3-Tridecene, (E)-        | 41446-57-5 | 128663   | -              | HC          | alkene              | 1474      | 0.295        | 69          | 1304         | NA           | 903           | 875            |
| Cinnamonicitrile         | 4360-47-8 | 672520   | -              | Nit         | nitrile             | 1474      | 0.96         | 129         | 1304         | 1301         | 928           | 917            |
| Naphthalene, 2-methyl-   | 91-57-6  | 1077813   | -              | HC          | polycyclic aromatic | 1478      | 0.54         | 142         | 1307         | 1307         | 948           | 942            |
| 2-Methyl-6-propylphenol  | 3520-52-3 | 44651     | -              | Oxy         | alcohol             | 1484      | 0.435        | 121         | 1310         | 1320         | 909           | 768            |
| 2,5-Diethylphenol        | 876-20-0 | 125693    | -              | Oxy         | alcohol             | 1488      | 0.43         | 135         | 1313         | 1313         | 882           | 810            |
| 1H-Inden-1-one, 2,3-dihydro-2-methyl- | 17496-14-9 | 68883   | -              | Oxy         | ketone              | 1490      | 0.76         | 131         | 1314         | NA           | 898           | 847            |
| 1-Ethyl-2-Heptylcyclopropane | 74663-86-8 | 30232     | -              | HC          | alicyclic HC        | 1492      | 0.295        | 70          | 1315         | NA           | 881           | 785            |
| 2-Methoxy-4-vinylphenol  | 7786-61-0 | 1673080   | M              | Oxy         | ether               | 1494      | 0.635        | 135         | 1316         | 1316         | 927           | 922            |
| p-Isopropenylacetophenone | 0604/5359 | 133698    | -              | Oxy         | ketone              | 1496      | 0.475        | 145         | 1318         | 1308         | 810           | 782            |
| Naphthalene, 1-methyl-   | 90-12-0  | 675002    | -              | HC          | polycyclic aromatic | 1504      | 0.53         | 142         | 1323         | 1323         | 946           | 936            |

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| Tentative Identification | CAS     | Peak Area | Health Effects | Class | Subclass | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|--------------------------|---------|-----------|----------------|-------|----------|----------|-----------|------------|---------|----------|----------|-------------|
| 5-Isopropenyl-2-methylcyclopent-1-ene carboxaldehyde | NA | 65082 | - | Oxy ketone | 1508 | 0.615 | 150 | 1325 | NA | 839 | 811 |
| 1-Methylindan-2-one | 35587-60-1 | 52433 | - | Oxy ketone | 1510 | 0.85 | 131 | 1327 | NA | 875 | 802 |
| 1-(3-Methylphenyl)4-methyl-3-pentene | 51082-26-9 | 112549 | - | HC aromatic | 1524 | 0.365 | 105 | 1335 | NA | 884 | 827 |
| Triacetin | 102-76-1 | 184532 | - | Oxy ester | 1528 | 1.145 | 103 | 1338 | 1339 | 959 | 949 |
| 4-Methylpyrrolo[1,2-alpyrazine | 64608-60-2 | 90679 | - | Nit nitrile | 1532 | 0.775 | 132 | 1340 | 1340 | 917 | 814 |
| 1H-Indenol | 56631-57-3 | 102269 | - | Oxy alcohol | 1538 | 0.53 | 132 | 1344 | NA | 909 | 825 |
| 1,5,9-Undecatriene, 2,6,10-trimethyl-, (Z)- | 62951-96-6 | 165119 | - | HC alkene | 1540 | 0.31 | 69 | 1345 | 1350 | 886 | 855 |
| Dodecane, 2,7,10-trimethyl- | 74645-98-0 | 273806 | - | HC alkane | 1544 | 0.335 | 57 | 1347 | NA | 862 | 751 |
| 3-Terpinolenone | 491-09-8 | 73662 | - | Oxy ketone | 1544 | 0.82 | 150 | 1347 | 1347 | 922 | 901 |
| Heptylcyclohexane | 5617-41-4 | 26543 | - | HC alicyclic | 1546 | 0.31 | 83 | 1348 | 1347 | 839 | 778 |
| Benzoic acid, 2-amino-, methyl ester | 134-20-3 | 650948 | - | Oxy ester | 1548 | 0.63 | 119 | 1350 | 1347 | 885 | 765 |
| Phenol, 2,6-dimethoxy- | 91-10-1 | 245761 | - | Oxy ether | 1552 | 0.71 | 154 | 1352 | 1352 | 918 | 912 |
| Eugenol | 97-53-0 | 75040 | G3 | Oxy alcohol | 1562 | 0.575 | 164 | 1358 | 1358 | 875 | 852 |
| Naphthalene, 1,2-dihydro-1,1,6-trimethyl- | 30364-38-6 | 144734 | - | HC polycyclic | 1570 | 0.41 | 142 | 1363 | 1364 | 870 | 833 |
| 3-Pyridinecarbonitrile, 1,4-dihydro- | 23974-91-6 | 290044 | - | Nit nitrile | 1576 | 1.04 | 105 | 1367 | NA | 905 | 774 |
| Benzene, heptyl- | 1078-71-3 | 181573 | - | HC monocyclic | 1578 | 0.37 | 92 | 1368 | 1369 | 885 | 855 |
| (Z)-8-Hydroxyinalool | 64142-78-5 | 326946 | - | Oxy alcohol | 1578 | 0.565 | 71 | 1368 | 1370 | 823 | 792 |
| Piperitenone oxide | 3564-96-3 | 130137 | - | Oxy epoxide | 1578 | 0.87 | 67 | 1368 | 1371 | 842 | 813 |

Continued on next page
Table S4. Tentatively identified compounds from the particulate phase fraction of mainstream marijuana smoke (Continued)

| Tentative Identification     | CAS      | Peak Area | Health Effects | Class         | Subclass          | 1<sub>t<sub>R (s) | 2<sub>t<sub>R (s) | Quant Mass | Exp. RI<sup>∗</sup> | Lib. RI<sup>∗</sup> | Reverse<sup>†</sup> | Similarity<sup>‡</sup> |
|------------------------------|----------|-----------|----------------|---------------|-------------------|------------------|------------------|-------------|------------------|------------------|-------------------|-------------------|
| Tridecane, 3-methyl-         | 6418-41-3| 61286     | -              | HC            | alkane            | 1582             | 0.295           | 57          | 1371             | 1371             | 843               | 815               |
| 1,3-Dimethyl-1H-indole       | 875-30-9 | 60390     | -              | Nit           | aza-arene         | 1588             | 0.625           | 144         | 1375             | 1383             | 865               | 785               |
| Farnesane                    | 3891-98-3| 486656    | -              | HC            | sesquiterpene     | 1590             | 0.305           | 71          | 1376             | 1376             | 929               | 919               |
| Germayl acetate              | 105-87-3 | 283776    | -              | Oxy           | ester             | 1592             | 0.485           | 69          | 1377             | 1377             | 905               | 897               |
| alpha-Ylangene               | 14912-44-8| 1052081   | -              | HC            | sesquiterpene     | 1596             | 0.35            | 105         | 1379             | 1379             | 922               | 920               |
| 1,13-Tetradecadiene          | 21964-49-8| 112649    | -              | HC            | alkene            | 1604             | 0.31            | 82          | 1384             | 1385             | 933               | 902               |
| Hexanoic acid, hexyl ester   | 6378-65-0| 175801    | -              | Oxy           | ester             | 1604             | 0.47            | 99          | 1384             | 1384             | 945               | 928               |
| 1,4-Dimethylazulene          | 1127-69-1| 37865     | -              | HC            | alicyclic         | 1606             | 0.52            | 141         | 1386             | 1390             | 875               | 772               |
| alpha-Copaene                | 3856-25-5| 284522    | -              | HC            | sesquiterpene     | 1606             | 0.345           | 119         | 1385             | 1384             | 940               | 926               |
| Biphenyl                     | 92-52-4  | 423669    | G2A            | HC            | polycyclic aromatic | 1612            | 0.48            | 154         | 1389             | 1391             | 934               | 922               |
| Quinoline, 4-methyl-1-Tetradecene | 491-35-0 | 31256     | M              | Nit           | aza-arene         | 1614             | 0.66            | 143         | 1391             | 1391             | 907               | 785               |
| alpha-Cubebene               | 17699-14-8| 321520    | -              | HC            | sesquiterpene     | 1618             | 0.3             | 69          | 1393             | 1393             | 951               | 941               |
| 1H-Pyrrole, 1-((4-methylphenyl)- | 827-60-1  | 41146      | -              | Het           | pyrrole           | 1622             | 0.52            | 157         | 1395             | NA               | 870               | 793               |
| 1H-Indole, 3-methyl-Tetradecane | 83-34-1  | 5674462   | -              | Nit           | aza-arene         | 1622             | 0.61            | 130         | 1395             | 1395             | 927               | 926               |
| 5-methyl-1H-Indole           | 629-59-4 | 1183079   | -              | HC            | alkane            | 1630             | 0.29            | 57          | 1400             | 1400             | 947               | 943               |
| 1-Ethynaphthalene            | 614-96-0 | 537250    | -              | Nit           | aza-arene         | 1634             | 0.625           | 130         | 1403             | 1397             | 903               | 896               |
| 2-Methylbiphenyl             | 643-58-3 | 28297     | X              | HC            | polycyclic aromatic | 1638            | 0.51            | 141         | 1406             | 1406             | 919               | 898               |
| Sesquithujene                | 159407-35-9| 339361   | -              | HC            | sesquiterpene     | 1640             | 0.315           | 119         | 1407             | 1408             | 922               | 915               |
| (+)-Sativene                 | 3650-28-0| 738704    | -              | HC            | sesquiterpene     | 1640             | 0.38            | 108         | 1407             | 1405             | 848               | 848               |
| trans-beta-Caryophyllene     | 87-44-5  | 162306    | -              | HC            | sesquiterpene     | 1654             | 0.37            | 93          | 1416             | 1416             | 943               | 925               |

<sup>∗</sup>Van Den Dool retention index (RI) relative to n-pentadecane = 1000;<br><sup>†</sup>Reverse similarity is calculated as 1-SIM;<br><sup>‡</sup>Similarity is calculated as 1-RCM.
| Tentative Identification                  | CAS     | Peak Area | Health Effects | Class | Subclass | $1_{TR}$ (s) | $2_{TR}$ (s) | Quant Mass | Exp. RI | Lib. RI | Reverse | Similarity |
|------------------------------------------|---------|-----------|----------------|-------|----------|--------------|--------------|------------|--------|--------|---------|------------|
| Naphthalene, 2,6-dimethyl-               | 581-42-0| 168521    | -              | HC    | polycyclic aromatic HC | 1656 | 0.53 | 156 | 1417 | 1416 | 928 | 896     |
| Naphthalene, 1,7-dimethyl-               | 575-37-1| 126413    | -              | HC    | polycyclic aromatic HC | 1660 | 0.525 | 156 | 1420 | 1419 | 942 | 910     |
| trans-alpha-Bergamotene                  | 17699-05-7| 769891    | -              | HC    | sesquiterpene | 1660 | 0.33 | 93  | 1420 | 1419 | 956 | 939     |
| beta-Copaene                             | 20479-06-5| 53597     | -              | HC    | sesquiterpene | 1662 | 0.36 | 120 | 1421 | 1422 | 852 | 827     |
| Naphthalene, 2-ethenyl-                  | 827-54-3| 75111     | -              | HC    | polycyclic aromatic HC | 1666 | 0.515 | 153 | 1424 | NA   | 917 | 799     |
| alpha-Santalene                          | 512-61-8| 639943    | -              | HC    | sesquiterpene | 1670 | 0.34 | 94  | 1426 | 1424 | 939 | 928     |
| (-)-Aristolene                           | 6831-16-9| 829626    | -              | HC    | sesquiterpene | 1674 | 0.355 | 105 | 1429 | 1429 | 877 | 877     |
| Naphthalene, 1,3-dimethyl-               | 575-41-7| 258060    | -              | HC    | polycyclic aromatic HC | 1678 | 0.525 | 141 | 1432 | 1427 | 914 | 905     |
| cis-beta-Caryophyllene                   | 118-65-0| 10066986  | -              | HC    | sesquiterpene | 1678 | 0.405 | 41  | 1431 | 1427 | 943 | 942     |
| N-methylphthalimide                      | 550-44-7| 110804    | -              | Nit imide | 1682 | 0.895 | 161 | 1434 | 1425 | 922 | 859     |
| Naphthalene, 1,5-dimethyl-               | 571-61-9| 372178    | -              | HC    | polycyclic aromatic HC | 1686 | 0.52 | 156 | 1437 | 1438 | 952 | 941     |
| gamma-Elemene                            | 339154-91-5| 142760  | -              | HC    | sesquiterpene | 1686 | 0.34 | 121 | 1437 | 1437 | 786 | 777     |
| cis-alpha-Bergamotene                    | 18252-46-5| 4752831  | -              | HC    | sesquiterpene | 1690 | 0.335 | 93  | 1439 | 1439 | 937 | 934     |
| alpha-Guaiene                            | 01/12/3691| 114731  | -              | HC    | sesquiterpene | 1698 | 0.345 | 105 | 1444 | 1444 | 851 | 832     |
| Sesquisabinene                           | 58319-04-3| 151396  | -              | HC    | sesquiterpene | 1702 | 0.34 | 69  | 1447 | 1444 | 818 | 800     |
| 3,5-Dimethoxy-4-hydroxytoluene           | 07/05/6638| 41316    | -              | Oxy ether | 1702 | 0.685 | 168 | 1447 | 1447 | 853 | 786     |
| Geranyl acetone                          | 3796-70-1| 306253    | -              | Oxy ketone | 1704 | 0.58  | 43  | 1448 | 1448 | 881 | 859     |
| Aromadendrene                            | 489-39-4| 837650    | -              | HC    | sesquiterpene | 1708 | 0.34 | 105 | 1451 | 1447 | 866 | 863     |
| **Continued on next page**               |         |           |                |       |          |              |              |            |        |        |         |            |
| Tentative Identification                          | CAS       | Peak Area | Health Effects | Class   | Subclass              | $t_R^1$ (s) | $t_R^2$ (s) | Quant Mass | Exp. RI$^*$ | Lib. RI$^*$ | Reverse$^1$ | Similarity$^1$ |
|------------------------------------------------|-----------|-----------|----------------|---------|-----------------------|-------------|-------------|------------|-------------|-------------|-------------|----------------|
| 1,4-Dimethylnaphthalene                         | 571-58-4  | 166033    | -              | HC      | polycyclic aromatic   | 1712        | 0.545       | 141        | 1454        | 1445        | 863         | 792            |
| trans-beta-Farnesene                            | 18794-84-8| 6043308   | -              | HC      | sesquiterpene         | 1712        | 0.325       | 69         | 1454        | 1453        | 941         | 937            |
| Isoeugenol                                      | 97-54-1   | 240482    | X              | Oxy     | alcohol               | 1714        | 0.605       | 164        | 1455        | 1455        | 945         | 920            |
| Alloaromadendrene                               | 25246-27-9| 493144    | -              | HC      | sesquiterpene         | 1722        | 0.355       | 161        | 1460        | 1461        | 899         | 897            |
| Metolcarb                                       | 1129-41-5 | 114387    | M              | Misc    | carbamate             | 1728        | 0.45        | 108        | 1464        | 1465        | 864         | 756            |
| Acenaphthylene                                  | 208-96-8  | 220557    | M              | HC      | polycyclic aromatic   | 1730        | 0.595       | 152        | 1465        | 1466        | 934         | 863            |
| cis-beta-Farnesene                              | 28973-97-9| 231849    | -              | HC      | sesquiterpene         | 1730        | 0.34        | 69         | 1465        | 1460        | 863         | 856            |
| (-)-Isolatede                                   | 95910-36-4| 150364    | -              | HC      | sesquiterpene         | 1732        | 0.37        | 133        | 1467        | NA          | 831         | 820            |
| 2(1H)-Pyridinone, 1-(3-oxy-1-cyclohexen-1-yl)   | 69914-13-2| 163091    | -              | Het     | pyridine              | 1734        | 0.37        | 133        | 1468        | NA          | 965         | 841            |
| alpha-Humulene                                  | 6753-98-6 | 2261781   | -              | HC      | sesquiterpene         | 1734        | 0.4         | 41         | 1468        | 1468        | 943         | 920            |
| Isoxadinene                                     | 16729-00-3| 63314     | -              | HC      | sesquiterpene         | 1736        | 0.35        | 159        | 1469        | 1472        | 814         | 761            |
| Valencene                                       | 03/07/4630| 269086    | -              | HC      | sesquiterpene         | 1736        | 0.365       | 133        | 1469        | 1467        | 809         | 808            |
| Bornyl butyrate                                 | 13109-70-1| 32081     | -              | Oxy     | ester                 | 1740        | 0.54        | 71         | 1472        | 1470        | 905         | 767            |
| epi-beta-Caryophyllene                          | 68832-35-9| 748493    | -              | HC      | sesquiterpene         | 1742        | 0.37        | 91         | 1473        | 1471        | 928         | 909            |
| Pyridine, 3-phenyl-                             | 1008-88-4 | 71024     | -              | Het     | pyridine              | 1746        | 0.62        | 155        | 1476        | 1470        | 907         | 828            |
| Diethylpropion (amfepramone)                    | 90-84-6   | 660488    | -              | Misc    | amphetamine           | 1748        | 1.15        | 100        | 1477        | 1477        | 749         | 634            |
| gamma-Murolene                                  | 30021-74-0| 1844412   | -              | HC      | sesquiterpene         | 1758        | 0.35        | 105        | 1483        | 1482        | 907         | 900            |
| 4-Dodecanol                                     | 10203-32-4| 35507     | -              | Oxy     | alcohol               | 1760        | 0.305       | 54         | 1485        | 1482        | 803         | 777            |
| gamma-Gurjunene                                 | 22567-17-5| 1163756   | -              | HC      | sesquiterpene         | 1764        | 0.355       | 91         | 1487        | 1487        | 909         | 894            |
| Benzonitrile, 2,4,6-trimethyl-trans-beta-Bergamotene| 2571-52-0| 1085818   | -              | Nit     | nitrile               | 1768        | 0.57        | 130        | 1490        | NA          | 856         | 849            |
| cis-murola-4(15),5-diene                        | 157477-72-0| 106835   | -              | HC      | sesquiterpene         | 1772        | 0.33        | 105        | 1492        | 1490        | 754         | 728            |

Continued on next page
| Tentative Identification | CAS     | Peak Area | Health Effects | Class | Subclass          | \( t_R \) (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|-------------------------|---------|-----------|----------------|-------|-------------------|---------------|------------|----------|----------|----------|-------------|
| 1,1'-Biphenyl, 4-methyl- | 644-08-6| 137194    | -              | HC    | polycyclic aromatic | 1776         | 0.47       | 168      | 1495     | 1492     | 928         | 906         |
| 4a,8-Dimethyl-2-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene | 103827-22-1 | 1212529 | -              | HC    | sesquiterpene      | 1776         | 0.36       | 133      | 1495     | 1492     | 933         | 915         |
| (-)-Myrtenol            | 19894-97-4 | 226589   | -              | Oxy   | alcohol            | 1776         | 0.37       | 108      | 1495     | NA       | 796         | 770         |
| alpha-Muurolene         | 5951-61-1  | 312165   | -              | HC    | sesquiterpene      | 1778         | 0.34       | 161      | 1496     | 1499     | 843         | 843         |
| Acenaphthene            | 83-32-9   | 64072    | G3             | HC    | polycyclic aromatic | 1780         | 0.52       | 153      | 1498     | 1496     | 930         | 916         |
| 2,3-dimethyl-1H-Indole  | 91-55-4   | 382997   | M              | Nit   | aza-arene          | 1782         | 0.645      | 144      | 1499     | 1507     | 926         | 908         |
| Pentadecane             | 629-62-9  | 1643950  | -              | HC    | alkane             | 1782         | 0.285      | 57       | 1499     | 1500     | 947         | 938         |
| (-)-Zingiberene         | 495-60-3  | 405932   | -              | HC    | sesquiterpene      | 1782         | 0.33       | 119      | 1499     | 1500     | 776         | 767         |
| beta-Selinene           | 17066-67-0 | 837908   | -              | HC    | sesquiterpene      | 1786         | 0.395      | 108      | 1502     | 1500     | 915         | 911         |
| alpha-Farnesene         | 502-61-4  | 1603821  | -              | HC    | sesquiterpene      | 1790         | 0.33       | 69       | 1504     | 1506     | 858         | 858         |
| (+)-Eremophilene        | NA       | 1275292  | -              | HC    | sesquiterpene      | 1790         | 0.355      | 161      | 1504     | 1504     | 897         | 895         |
| alpha-Selinene          | 473-13-2  | 3367916  | -              | HC    | sesquiterpene      | 1794         | 0.375      | 93       | 1507     | 1508     | 946         | 939         |
| 1-Naphthalenecarbonitrile | 86-53-3  | 88851    | M              | Nit   | nitrile            | 1796         | 0.86       | 153      | 1509     | 1503     | 900         | 797         |
| Naphthalene, 1-butyl-1,2,3,4-tetrahydro-beta-Bisabolene | 38857-76-0 | 1200430 | -              | HC    | alicyclic          | 1798         | 0.455      | 131      | 1510     | 1518     | 781         | 781         |
| delta-Cadinene          | 495-61-4  | 2956361  | -              | HC    | sesquiterpene      | 1802         | 0.32       | 69       | 1513     | 1511     | 890         | 890         |
| Sesquicinol             | 483-76-1  | 944522   | -              | HC    | sesquiterpene      | 1802         | 0.335      | 161      | 1513     | NA       | 837         | 830         |
| beta-Cadinene           | 90131-02-5 | 213493   | -              | Oxy   | alcohol            | 1812         | 0.37       | 139      | 1520     | 1520     | 811         | 808         |
| delta-Cadinene          | 523-47-7  | 1522493  | -              | HC    | sesquiterpene      | 1822         | 0.33       | 161      | 1527     | 1523     | 866         | 864         |
| Germacrene B            | 15423-57-1 | 2172288  | -              | HC    | sesquiterpene      | 1822         | 0.35       | 121      | 1527     | 1523     | 795         | 783         |
| beta-Sesquiphellandrene | 20307-83-9 | 1007655  | -              | HC    | sesquiterpene      | 1826         | 0.35       | 69       | 1529     | 1525     | 943         | 906         |
| Bibenzyl                | 103-29-7  | 757715   | -              | HC    | polycyclic aromatic| 1828         | 0.45       | 91       | 1531     | 1528     | 915         | 902         |

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| Tentative Identification | CAS     | Peak Area | Health Effects | Class Subclass | 1<sub>τ</sub><sub>R</sub> (s) | 2<sub>τ</sub><sub>R</sub> (s) | Quant Mass | Exp. RI<sup>∗</sup> | Lib. RI<sup>∗</sup> | Reverse† | Similarity‡ |
|-------------------------|---------|-----------|----------------|----------------|----------------|---------------|-------------|----------------|----------------|-----------|-----------|
| trans-Calamene          | 73209-42-4 | 500790   | -              | HC sesquiterpene | 1828          | 0.38          | 159         | 1531           | 1529           | 864      | 854       |
| 1-Naphthol              | 90-15-3   | 60444    | X              | Oxy alcohol     | 1828          | 0.56          | 144         | 1531           | 1525           | 895      | 804       |
| (-)-Eremophiline        | 10219-75-7 | 1989151  | -              | HC sesquiterpene | 1830          | 0.37          | 161         | 1532           | 1541           | 892      | 887       |
| Dibenzofuran            | 132-64-9  | 193780   | M              | Het furan       | 1832          | 0.56          | 168         | 1534           | 1532           | 854      | 817       |
| Naphthalene, 1,4,5-trimethyl- | 2131-41-1 | 66058   | -              | HC aromatic poly cyclic aromatic HC | 1838          | 0.505         | 155         | 1538           | 1535           | 875      | 825       |
| alpha-Gurjunene         | 489-40-7  | 1231424  | -              | HC sesquiterpene | 1846          | 0.34          | 204         | 1543           | NA             | 858      | 854       |
| Naphthalene, 2,3,6-trimethyl- | 829-26-5  | 218894   | -              | HC poly cyclic aromatic HC | 1848          | 0.505         | 155         | 1545           | 1550           | 923      | 905       |
| trans-alpha-Bisabolene  | 25532-79-0 | 5867866  | -              | HC sesquiterpene | 1848          | 0.31          | 93          | 1545           | 1540           | 919      | 909       |
| Pyridine, 4-(1-pyrrolidinyl)alpha-Cadinene | 24406-05-1 | 357461   | -              | Het pyridine    | 1850          | 0.775         | 147         | 1546           | NA             | 881      | 750       |
| alpha-Calacorene        | 21391-99-1 | 1088877  | -              | HC sesquiterpene | 1860          | 0.39          | 105         | 1548           | 1546           | 850      | 845       |
| Selina-3,7(11)-diene    | 6813-21-4  | 1819658  | -              | HC sesquiterpene | 1864          | 0.37          | 204         | 1555           | 1545           | 910      | 908       |
| Ochracin                | 17397-85-2 | 72999    | -              | Oxy lactone     | 1866          | 1            | 134         | 1558           | NA             | 851      | 790       |
| Naphthalene, 1,4,6-trimethyl- | 2131-42-2 | 106267   | -              | HC poly cyclic aromatic HC | 1868          | 0.505         | 155         | 1559           | NA             | 809      | 752       |
| Nerolidol               | 40716-66-3 | 1247143  | -              | Oxy alcohol     | 1874          | 0.39          | 93          | 1563           | 1564           | 920      | 919       |
| Phenol, 4-ethenyl-2,6-dimethoxy- | 28343-22-8 | 95679    | -              | Oxy ether       | 1880          | 0.67          | 180         | 1567           | 1568           | 901      | 855       |
| Pentadecane, 3-methyl-   | 2882-96-4  | 111179   | -              | HC alkane       | 1884          | 0.29          | 57          | 1570           | 1569           | 855      | 815       |
| Benzene, nonyl-         | 1081-77-2  | 102398   | -              | HC monocyclic aromatic HC | 1892          | 0.365         | 92          | 1575           | 1576           | 808      | 752       |
| cis-6-Eudesmen-11-ol    | 194607-96-0 | 99512    | -              | Oxy alcohol     | 1892          | 0.48          | 59          | 1575           | 1566           | 852      | 830       |
| Germacrene D-4-ol       | 198991-79-6 | 342520   | -              | Oxy alcohol     | 1906          | 0.47          | 43          | 1585           | 1579           | 830      | 814       |
| 1-Hexadecene            | 629-73-2   | 221613   | -              | HC alkene       | 1916          | 0.295         | 83          | 1592           | 1592           | 940      | 938       |

Continued on next page
| Tentative Identification | CAS       | Peak Area | Health Effects | Class      | Subclass              | $t_R$ (s) | $t_R$ (s) | Quant Mass | Exp. RI$^*$ | Lib. RI$^*$ | Reverse$^1$ | Similarity$^1$ |
|--------------------------|-----------|-----------|----------------|------------|-----------------------|----------|----------|------------|------------|------------|-------------|----------------|
| 3,5,11-Eudesmatriene     | 193615-07-5 | 119580    | -              | HC         | sesquiterpene         | 1920     | 0.36     | 187        | 1595       | NA         | 874          | 866            |
| beta-Caryophyllene oxide | 1139-30-6  | 1043419   | -              | Oxy        | epoxide               | 1924     | 0.665    | 79         | 1598       | 1596       | 945          | 945            |
| Hexadecane               | 544-76-3   | 597530    | X              | HC         | alkane                | 1926     | 0.285    | 57         | 1599       | 1600       | 942          | 941            |
| Fluorene                 | 86-73-7    | 217051    | G3             | HC         | polycyclic            | 1928     | 0.545    | 166        | 1600       | 1604       | 935          | 922            |
| Viridiflorol             | 552-02-3   | 92975     | -              | Oxy        | alcohol               | 1930     | 0.465    | 43         | 1602       | 1601       | 804          | 756            |
| 3-Hexadecene, (Z)-       | 34303-81-6 | 93822     | -              | HC         | alkene                | 1932     | 0.285    | 55         | 1603       | 1604       | 916          | 849            |
| Champacol                | 13822-35-0 | 252025    | -              | Oxy        | alcohol               | 1936     | 0.45     | 59         | 1606       | 1602       | 884          | 878            |
| Humulene epoxide 1       | 19888-33-6 | 118018    | -              | Oxy        | epoxide               | 1946     | 0.63     | 93         | 1614       | 1610       | 874          | 852            |
| Humulene epoxide 2       | 19888-34-7 | 393487    | -              | Oxy        | epoxide               | 1962     | 0.645    | 96         | 1626       | 1620       | 918          | 917            |
| beta-Vetivenene          | 27840-40-0 | 170951    | -              | HC         | sesquiterpene         | 1964     | 0.365    | 187        | 1627       | NA         | 879          | 874            |
| alpha-Muurolol           | 19912-67-5 | 27353     | -              | Oxy        | alcohol               | 1966     | 0.45     | 119        | 1629       | 1626       | 849          | 826            |
| Selin-6-en-4-alpha-ol    | 118173-08-3| 778591    | -              | Oxy        | alcohol               | 1978     | 0.485    | 81         | 1638       | 1636       | 875          | 864            |
| gamma-Eudesmol           | 1209-71-8  | 417823    | -              | Oxy        | alcohol               | 1988     | 0.465    | 59         | 1645       | 1642       | 855          | 838            |
| Pentadecane, 2,6,10-trimethyl- | 3892-00-0 | 444915    | -              | HC         | alkane                | 1990     | 0.3      | 57         | 1647       | 1649       | 910          | 903            |
| Hexanoic acid, 2-phenylethyl ester | 6290-37-5 | 81090     | -              | Oxy        | ester                 | 1990     | 0.525    | 104        | 1647       | 1649       | 848          | 761            |
| (-)-Cubenol              | 21284-22-0 | 35271     | -              | Oxy        | alcohol               | 1992     | 0.46     | 179        | 1648       | 1642       | 839          | 814            |
| cis-Lanceol              | 10067-29-5 | 113386    | -              | Oxy        | alcohol               | 2014     | 0.465    | 187        | 1665       | NA         | 802          | 790            |
| alpha-Cadinol            | 481-34-5   | 127624    | -              | Oxy        | alcohol               | 2020     | 0.465    | 95         | 1669       | 1669       | 855          | 815            |
| beta-Atlantol            | 38142-56-2 | 150890    | -              | Oxy        | alcohol               | 2022     | 0.45     | 187        | 1671       | NA         | 823          | 807            |
| beta-Eudesmol            | 473-15-4   | 833555    | -              | Oxy        | alcohol               | 2024     | 0.495    | 59         | 1672       | 1674       | 892          | 882            |
| Bisabolene oxide A       | NA        | 390747    | -              | Oxy        | epoxide               | 2028     | 0.505    | 43         | 1675       | 1672       | 793          | 772            |
| 8-Heptadecene            | 16369-12-3 | 126569    | -              | HC         | alkene                | 2034     | 0.295    | 69         | 1679       | 1680       | 870          | 841            |
| Bulnesol                 | 22451-73-6 | 177808    | -              | Oxy        | alcohol               | 2034     | 0.455    | 107        | 1679       | 1668       | 910          | 903            |
| 1-Heptadecene            | 6765-39-5  | 235035    | -              | HC         | alkene                | 2052     | 0.3      | 57         | 1693       | 1692       | 928          | 910            |
| Tentative Identification                  | CAS    | Peak Area | Health Effects | Class | Subclass | $t_{1R}$ (s) | $t_{2R}$ (s) | Quant Mass | Exp. RI* | Lib. RI* | Reverse† | Similarity‡ |
|------------------------------------------|--------|-----------|----------------|-------|----------|--------------|--------------|------------|----------|----------|----------|-------------|
| alpha-Bisabolol                          | 515-69-5 | 1515188   | -              | Oxy   | alcohol  | 2054         | 0.41         | 119        | 1694     | 1695     | 946       | 920         |
| 2-Pentadecanone                          | 2345-28-0 | 87941     | -              | Oxy   | ketone   | 2060         | 0.54         | 58         | 1699     | 1699     | 933       | 838         |
| Heptadecane                              | 629-78-7 | 651123    | -              | HC    | alkane   | 2062         | 0.29         | 57         | 1700     | 1700     | 948       | 932         |
| Pristane                                 | 1921-70-6 | 147651    | X              | HC    | alkane   | 2068         | 0.305        | 57         | 1705     | 1707     | 885       | 871         |
| Juniper Camphor                          | 473-04-1 | 1295466   | -              | Oxy   | alcohol  | 2082         | 0.465        | 43         | 1716     | NA       | 898       | 897         |
| 9H-Fluorene, 1-methyl-                    | 1730-37-6 | 88338     | -              | HC    | -        | 2084         | 0.535        | 165        | 1717     | 1719     | 926       | 859         |
| Isospathulenol                           | 88395-46-4 | 361161    | -              | Oxy   | alcohol  | 2096         | 0.44         | 43         | 1727     | NA       | 847       | 844         |
| 3-Methyl-5-(2,6,6-trimethyl-1-cyclohexen-1-yl)-1-pentyn-3-ol | 5417-74-3 | 47576     | -              | Oxy   | alcohol  | 2102         | 0.635        | 55         | 1731     | NA       | 792       | 769         |
| Geranyl hexanoate                        | 10032-02-7 | 542521    | -              | Oxy   | ester    | 2126         | 0.425        | 69         | 1750     | 1756     | 912       | 912         |
| Olivetol                                 | 500-66-3 | 1023266   | M              | Oxy   | alcohol  | 2158         | 0.525        | 124        | 1774     | 1771     | 899       | 878         |
| alpha-Muurolene-14-ol                    | 81968-62-9 | 159779    | -              | Oxy   | alcohol  | 2178         | 0.455        | 91         | 1790     | 1781     | 802       | 754         |
| 5-Octadecene, (E)-                      | 7206-21-5 | 163652    | -              | HC    | alkene   | 2184         | 0.3         | 57         | 1794     | NA       | 931       | 927         |
| Octadecane                               | 593-45-3 | 333781    | -              | HC    | alkene   | 2192         | 0.29         | 57         | 1800     | 1800     | 908       | 903         |
| Anthracene                               | 120-12-7 | 113566    | G3             | HC    | -        | 2202         | 0.615        | 178        | 1809     | 1802     | 937       | 878         |
| 2-Phytene (cis)                          | NA     | 276471    | -              | HC    | alkene   | 2230         | 0.31         | 70         | 1831     | 1835     | 882       | 869         |
| Neophytadiene                            | 504-96-1 | 2346734   | -              | HC    | diterpene | 2238        | 0.335        | 68         | 1838     | 1838     | 931       | 919         |
| 2-Phytene (trans)                        | 2437-93-6 | 554433    | -              | HC    | alkene   | 2244         | 0.31         | 70         | 1843     | 1838     | 893       | 889         |
| 2-Pentadecanone, 6,10,14-trimethyl-       | 502-69-2 | 324771    | -              | Oxy   | ketone   | 2244         | 0.545        | 58         | 1843     | 1843     | 894       | 875         |
| 1-Nonadecene                             | 18435-45-5 | 97546     | -              | HC    | alkene   | 2306         | 0.305        | 83         | 1894     | 1893     | 926       | 903         |
| Nonadecane                               | 629-92-5 | 258567    | -              | HC    | alkene   | 2314         | 0.295        | 57         | 1900     | 1900     | 933       | 921         |
| beta-Springene                           | 70901-63-2 | 655600    | -              | HC    | alkene   | 2330         | 0.33         | 69         | 1914     | NA       | 893       | 882         |
| trans,trans-Farnesyl acetone             | 762-29-8 | 117190    | -              | Oxy   | ester    | 2330         | 0.53         | 43         | 1914     | 1914     | 862       | 814         |

Continued on next page
| Tentative Identification                                      | CAS      | Peak Area | Health Effects | Class          | Subclass     | $t_R$ (s) | $2t_R$ (s) | Quant | Exp. RI | Lib. RI | Reverse† | Similarity‡ |
|--------------------------------------------------------------|----------|-----------|----------------|----------------|--------------|-----------|-----------|-------|---------|---------|----------|-------------|
| Hexadecanoic acid, methyl ester                             | 112-39-0 | 664110    |                | Oxy ester      |              | 2344      | 0.42      | 74    | 1926    | 1926    | 954      | 911        |
| gamma-Camphorene                                            | 20016-73-3 | 185632    |                | HC diterpene   |              | 2378      | 0.33      | 69    | 1955    | 1960    | 818      | 810        |
| alpha-Springene                                             | 77898-97-6 | 165741    |                | HC alkene      |              | 2390      | 0.335     | 69    | 1965    | 1969    | 857      | 836        |
| Cyclo-L-leu-L-pro                                           | 5654-86-4 | 162198    |                | Nit amino acid |              | 2390      | 1.26      | 154   | 1966    | NA      | 853      | 795        |
| Cycro-(Pro-Pro)                                             | 19943-27-2 | 547300    |                | Nit amino acid |              | 2396      | 1.19      | 70    | 1971    | NA      | 937      | 842        |
| alpha-Camphorene                                            | 20016-72-2 | 66922     |                | HC diterpene   |              | 2420      | 0.33      | 69    | 1990    | 1994    | 825      | 780        |
| Hexadecanoic acid, ethyl ester                             | 628-97-7 | 116092    |                | Oxy ester      |              | 2422      | 0.42      | 88    | 1992    | 1990    | 936      | 874        |
| 1-Heptadecanol                                              | 1454-85-9 | 48717     |                | Oxy alcohol    |              | 2424      | 0.31      | 83    | 1994    | 1986    | 905      | 877        |
| Eicosane                                                    | 112-95-8 | 171899    |                | HC alkane      |              | 2432      | 0.3       | 57    | 2000    | 2000    | 906      | 893        |
| Heneicosane                                                 | 629-94-7 | 133774    |                | HC alkane      |              | 2544      | 0.305     | 57    | 2100    | 2100    | 927      | 906        |
| 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-       | 301-00-8 | 147680    |                | Oxy ester      |              | 2544      | 0.445     | 79    | 2100    | 2100    | 878      | 850        |
| Methyl 9-octadecenoate                                      | 1937-62-8 | 39096     |                | Oxy ester      |              | 2550      | 0.43      | 74    | 2106    | 2107    | 926      | 878        |
| Phytol                                                      | 150-86-7 | 214271    |                | Oxy alcohol    | polycyclic   | 2562      | 0.43      | 71    | 2117    | 2117    | 901      | 866        |
| Pyrene                                                      | 129-00-0 | 35113     | G3             | HC             | aromatic     | 2604      | 0.69      | 202   | 2157    | NA      | 913      | 807        |
| Linoleic acid ethyl ester                                   | 544-35-4 | 35937     |                | Oxy ester      |              | 2608      | 0.44      | 67    | 2161    | 2159    | 831      | 778        |
| Hexadecanamide                                              | 629-54-9 | 266783    |                | Nit amide      |              | 2636      | 0.685     | 59    | 2187    | 2186    | 768      | 738        |
| 1-Docosene                                                  | 1599-67-3 | 41488     |                | HC alkene      |              | 2644      | 0.315     | 57    | 2195    | 2194    | 911      | 881        |
| Docosane                                                    | 629-97-0 | 104426    |                | HC alkane      |              | 2650      | 0.31      | 57    | 2200    | 2200    | 914      | 844        |
| trans-Ferruginol                                            | 514-62-5 | 978408    |                | Oxy alcohol    |              | 2780      | 0.49      | 203   | 2326    | 2325    | 761      | 761        |
| Cannabivarin                                                | 33745-21-0 | 74634     |                | Oxy cannabinoid |              | 2840      | 0.54      | 267   | 2383    | 2383    | 835      | 760        |
| Cannabidiol                                                 | 521-37-9 | 695605    | M              | Oxy cannabinoid |              | 2882      | 0.495     | 231   | 2424    | NA      | 818      | 815        |
| 3-t-Butyl-6,6,9-trimethyl-6a,7,10a-tetrahydro-6H-benzo[e]chromen-1-ol | NA | 250952 | - | Oxy alcohol | 2884 | 0.485 | 217 | 2426 | NA | 790 | 776 |
| Cannabichromene                                            | 20675-51-8 | 5405025 | M | Oxy cannabinoid | 2888 | 0.46 | 231 | 2429 | NA | 900 | 891 |
| Tentative Identification                          | CAS       | Peak Area | Health Effects | Class       | Subclass        | $t_R$ (s) | $2t_R$ (s) | Quant Mass | Exp. RI $^*$ | Lib. RI $^*$ | Reverse $^*$ | Similarity $^*$ |
|------------------------------------------------|-----------|-----------|----------------|-------------|----------------|----------|----------|------------|-------------|-------------|--------------|----------------|
| delta-8-Tetrahydrocannabinol                     | 5957-75-5 | 613499    | M              | Oxy         | cannabinoid    | 0.46     | 231      | 2493       | NA          | 901         | 898          |
| 11-Hydroxy-delta-9-tetrahydrocannabinol          | 36557-05-8| 149971    | M              | Oxy         | cannabinoid    | 0.5      | 299      | 2506       | NA          | 774         | 764          |
| delta-9-Tetrahydrocannabinol                     | 03/08/1972| 33950035  | M              | Oxy         | cannabinoid    | 0.55     | 231      | 2520       | NA          | 790         | 774          |
| Cannabigerol                                     | 25654-31-3| 761069    | -              | Oxy         | cannabinoid    | 0.5      | 115      | 2566       | NA          | 908         | 896          |
| Cannabinol                                       | 521-35-7  | 945625    | M              | Oxy         | cannabinoid    | 0.57     | 310      | 2574       | NA          | 812         | 781          |
| Octacosane (no library hit)                     | 630-02-4  | 75282     | HC             | alkane      | 3274          | 0.4      | 57       | 2800       | 2800        | 902         | 845          |
| Octacosane, 2-methyl-                            | 1560-98-1 | 346200    | -              | HC          | alkane        | 3352     | 0.45     | 57         | 2875        | 2866        | 856          | 842          |
| Tetracosyl benzoate                              | 103569-99-9| 325500  | -              | Oxy         | ester         | 1.59     | 123      | 3005       | NA          | 863         | 753          |
| Vitamin E                                        | 10191-41-0| 219745    | -              | Oxy         | alcohol       | 0.79     | 165      | 3024       | NA          | 835         | 817          |

$^*$RI is Kovats Retention Index. "Exp. RI" refers to an experimental retention index calculated for this analysis. "Library RI" refers to a tabulated RI value obtained from NIST, PubChem, or ChemSpider electronic sources.

$^1$Similarity refers to a "forward" mass spectral match score (i.e., how well does an experimentally-obtained spectrum fit to a library entry). In the case of a forward search, the match score (out of a maximum of 1000) for the experimental spectrum is penalized for containing extra peaks that are not present in the library spectrum.

$^2$Reverse refers to a "backwards" mass spectral match score (i.e., how well does a library entry fit to an experimentally-obtained spectrum). A reverse search match score (out of a maximum of 1000) for the library spectrum is not penalized for having extra peaks not contained in the experimental spectrum. A reverse search only requires that peaks in the library spectrum are present in the experimental spectrum.

Health effects were classified using the International Agency for Research on Cancer (IARC) carcinogen list and the Registry of Toxic Effects of Chemical Substances (RTECS) provided by the Canadian Centre for Occupational Health and Safety (CCOHS).

G1 = Group 1 carcinogen, G2A = Group 2A carcinogen, G2B = Group 2B carcinogen, G3 = Group 3 carcinogen, M = mutagen, T = teratogen, X = toxic by other mechanisms, "-" = no risk data available/risks mitigated by proper protective equipment.

NA = not available, HC = hydrocarbon, Het = heterocycle, Misc = miscellaneous, Nit = nitrogenated, Oxy = oxygenated
SPME-GCxGC-TOFMS methods
GERSTEL MAESTRO Method

C:\ProgramData\Gerstel\Maestro\1\Methods\Tob-Cannb.1.mth

Method Information

No Method Information

Global Parameters

| Parameter         | Value   |
|-------------------|---------|
| Runtime           | 60.00 min |
| Cool Down Time    | 7.00 min  |
| Cryo Timeout      | 15.00 min |
MPS SPME Injection

Syringe Parameters
Syringe: Fiber SPME

Sample Preparation
SPME from Tray: disabled
Incubator: Agitator 1
Incubation Temp.: 70 °C
Incubation Time: 3.00 min
Agitator On Time: 10 s
Agitator Off Time: 1 s
Agitator Speed: 250 rpm

Sample Parameters
Sample Tray Type: VT15/20-CVM
Vial Penetration: 43.00 mm
Extraction Time: 15.00 min
Inj. Penetration: 54.00 mm
Desorption Time: 120 s

Fiber Bakeout
Bakeout at: NONE

Derivatisation
Derivatisation Mode: No Derivatisation

Information
Hardware control:
- Agilent© 7890 Agilent© 7890 Gas Chromatograph
- Agilent© 6890 Agilent© 6890 Gas Chromatograph
- Shimadzu© GC-2010 Shimadzu© GC-2010
- Generic Generic Gas Chromatograph
- Direct Inlet Direct Inlet to Calibration Compound

Option:
- ☐ MACH/LTM Oven
- ☑ LECO© GCxGC

Capillary Configuration:
No problems detected with column configuration.

Flow Path 1:

| # | Type     | Location  | Length(m) | Int. Diameter(μ) | Max Temp | Film Thickness | Phase   | Bleed Masses |
|---|----------|-----------|-----------|------------------|----------|----------------|---------|--------------|
| 1 | Inlet    | Front     |           |                  |          |                |         |              |
| 2 | Capillary | GC Oven   | 60.000    | 250.00           | 350.0    | 0.25           | Rtx-5Sil| 73 149 207 281 |
| 3 | Capillary | Modulator | 0.100     | 250.00           | 340.0    | 0.25           | Rtx-200l| 73 149 207 281  |
| 4 | Capillary | Secondař  | 1.290     | 250.00           | 340.0    | 0.25           | Rtx-200l|              |
| 5 | Capillary | Detector  | 0.210     | 250.00           | 340.0    | 0.25           | Rtx-200l|              |
| 6 | Detector | TOF       |           |                  |          |                |         |              |

Mass Selection for Auto Mass Defect Tracking
- ☑ Excluded Masses in Auto Mass Defect Mode (Set Auto Mass Defect Mode in MS method. Select masses between 130 to 384 inclusive.)
- For general unknown analyses. Select column bleed, matrix, interfering, and non-target masses.
- ☑ Included Masses in Auto Mass Defect Mode (Generally for target analyses. Select significant masses of target analytes, minimum of 2 masses required.)
Carrier Gas:
Helium

Front Inlet Type:
Split / Splitless

Front Inlet Mode:
Split

Active Inlet Location:
☒ Front  ☐ Back  The active inlet must be present in the capillary configuration.

No problems detected with pressure / flow.

☑ Corrected constant flow via pressure ramps  Use this mode when in GCxGC mode or using short ( < 5 m ) single column or two columns.

| # | Rate (mL/min²) | Target Flow (mL/min) | Duration (min) |
|---|---|---|---|
| 1* | Initial | 2.00 | Entire Run |

Front Inlet Septum Purge Flow (mL/min):
3  0 - 30 mL/min

Column 1 / Front Inlet Split Ratio:
20 The ratio of split flow to column flow. This value cannot be used if your column is not defined (i.e. length, diameter, thickness).

Column 1 / Front Inlet Split Flow (mL/min):
40 Represents the flow from the split/purge vent. This value cannot be used if your column is not defined.
Column 1 / Front Inlet Total Flow (mL/min):

This is the total flow into the inlet, which is the sum of the split flow, and column flow. It does not include the septum purge flow. When the total flow is changed, the split ratio and split flow change while the column flow and pressure remain the same.

| Column 1 / Front Inlet Gas Saver | Yes | No |
|----------------------------------|-----|----|

Column 1 / Front Inlet Gas Saver Flow (mL/min):

15

Column 1 / Front Inlet Gas Saver Time (minutes):

3.5

Front Inlet temperature(s):

| #  | Rate (°C/min) | Target Temp (°C) | Duration (min) |
|----|---------------|------------------|----------------|
| 1* | Initial       | 250              | Entire Run     |

No problems detected with oven temperatures.

Oven Equilibration Time (sec):

10

Enter oven temperature ramp below:

| #  | Rate (°C/min) | Target Temp (°C) | Duration (min) |
|----|---------------|------------------|----------------|
| 1* | Initial       | 50               | 5.00           |
| 2  | 5.00          | 300              | 5.00           |

Coolant to Column Oven: On

Enable Secondary Oven

Secondary Oven Temperature Offset (°C, relative to the GC oven temperature):
+5 °C is recommended

Use Advanced Secondary Temperature Programming

☑ Modulator Enabled

Modulator Temperature Offset ( °C, relative to the secondary oven temperature):
+15 °C is recommended

☐ Use Advanced Modulator Temperature Programming

Purge Pulse Time ( sec):
0

Modulation Timing:
For 1D GC set second dimension time to 0

| #  | Start          | End           | Modulation Period (s) | Hot Pulse Time | Cool Time Between Stages |
|----|----------------|---------------|------------------------|----------------|--------------------------|
| 1  | Start of Run   | End of Run    | 2.00                   | 0.30           | 0.70                     |

Transfer Line Temperature Equilibration Time ( sec ):
0

Transfer Line Temperature ( °C ):
250
Specify Additional Detectors & Auxiliary Pneumatics
Use GC method total time for MS method total time:
- Yes
- No

**Acquisition delay**
- 30 Sec.
- 30 Min.

The length of time from injection until the data system will start storing data from the mass spectrometer.

Enter time(s) when the filament should be turned off (min of 3 sec) in the grid below

| #  | Start             | End    | Filament |
|----|-------------------|--------|----------|
| 1* | Start of Run      | 30 s   | Off      |
| 2  | 30 s              | End of Run | On      |

Required Disk Space
- NA

Enter the mass spectrometer settings:

**Start Mass (u)**
- 40

**End Mass (u)**
- 500

**Acquisition Rate (spectra/second)**
- 200

**Detector Voltage:**
- Specify Relative Detector Voltage

- **Optimized Voltage**: 200
- **Offset**: 200

**Electron Energy (Volts)**
- -70

**Mass defect mode**
- Auto (Select masses for automatic tracking in column information section of GC method.)
- Manual

- **Verify offset before collecting data**

**Mass Defect (mu/100 u)**
- 0
Set the temperature for the Ion Source:

| Ion Source (°C) | 200 |

- Wait for ion source temperatures to reach set point before starting acquisition

**Source Temperature Equilibration Time (Seconds)**

| 0 |

**Enter the masses to display during acquisition**

- **Examples**
  - t TIC
  - 69,131 Masses 69 and 131
  - 69+131 Sum of masses 69 and 131
Select the task or tasks you wish to perform from the list below:

- Baseline - computes baseline
- Peak Find - finds peaks above the baseline using TSD®
- Library Search - identifies all peaks found
- Calculate Area / Height - computes the area and height of peaks without a calibration
- Retention Index Method
- Classifications
- Apply Calibration(s) - computes the absolute concentration of peaks based upon a calibration
- Apply Reference(s) - computes the relative concentration of peaks with respect to a reference
- Semi Quantification - computes concentration based on another analytes calibration curve
- Tune Check
- Tailing Factor Check - checks to see if the analytes have an acceptable peak shape
- Calibration Check
- Blank Check - checks to make sure none of the analytes exceed their blank concentration
- Report - prints selected reports for each sample
- Export peak information in ASCII CSV format
- Export data in Andi MS format (.cdf)
- Export data file
- Cache script results

---

Enter baseline tracking info below:

|   | Start | End | Mode |
|---|-------|-----|------|
| 1* | Start of Run | End of Run | Default |

Add
Remove

Enter the baseline offset below (0.5-3.0):

Examples:
- 0.5: Through the middle of the noise
- 1.0: Just above the noise

Enter the number of data points that should be averaged for smoothing below:

Auto

---

GCxGC Parameters

1st Dimension

Enter the expected peak width in seconds below.

Peak widths broaden throughout the chromatographic run: 12

Peak Width values should be the expected number of slices multiplied by the modulation period. Typically, 3 to 6 slices per...
2nd Dimension

Match Required to combine: 750

Override the allowed second dimension R.T shift for combine

Early

Late

Enter the expected peak width in seconds below: (as measured from baseline to baseline)

Peak widths broaden throughout the chromatographic run

For broadening, two peak widths may be specified at two different retention times. All peak widths will be extrapolated from these two points.

Add... Remove

Filter peaks by classification

Enter the minimum required S/N for the subpeak to be retained.

Integration Approach:

Traditional

Adaptive

Keep False Peaks

Enter segmented processing info below:

| # | Start | End | Peak Find | S/N | Masses | Number of Apexing Masses |
|---|-------|-----|-----------|-----|--------|--------------------------|
| 1* | Start of Run | End of Run | On | 100.0 | 4 |
Common masses in derivatized products:

Library Identity Search Mode:
- Normal
- Quick

Library Search Mode:
- Forward
- Reverse

Enter the number of library hits to return:

Enter the masses to library search below:

Minimum molecular weight allowed:

Maximum molecular weight allowed:

Mass Threshold (Relative abundance of base ion (0 - 998))

Minimum similarity match before name is assigned (0 - 999)

Add the libraries to use for searching below:

- mainlib
- replib
- W8N08

Enable Additional Library Search Criteria

Add skimming off small riding peaks
Select the retention index method to convert retention time to retention index:

**Ryan_Ben.Retention Index**  
**Select ...**

- **Check Retention Index Analytes**
  
  **Criteria:**
  
  - Maximum allowed retention index variation. **10**

  **Options:**
  
  - Update the retention times of retention index analytes.

Select directory and columns to export below:

- **Directory**
  
  **G:\Cannabis Smoke-CSV\**  
  **Browse...**

- **Remove repetition from sample name when generating filename**

**Header:** (Leave Blank if no header information is desired)

- **Functions...**

**Field Separator**

- **Comma**
- **Tab**

**Filter**

- **Calculate area percentage from filtered peaks only**

- **Quantifieds**
  
  - **Analytes**
  - **Surrogates**
  - **Internal Standards**

- **Match**

- **Out of Tolerance**

- **Contaminants / Unknowns**

- **Not Founds**

- **Group:**  
  
  **Classifications:**
| Group                  | Height | Hit | Hit # | IntegrationBegin | IntegrationEnd | Ion Ratio Mass 1 Response 1 | Ion Ratio Mass 1 Response 2 | Ion Ratio Mass 1 Response 3 | Ion Ratio Mass 2 Response 1 | Ion Ratio Mass 2 Response 2 | Ion Ratio Mass 2 Response 3 | Ion Ratio Masses 1 | Ion Ratio Masses 2 | Ion Ratio Masses 3 | Ion Ratio Result 1 | Ion Ratio Result 2 | Ion Ratio Result 3 | Mass Defect | Noise | Non-Saturated Apex (s) | Peak Number | Probability | Profile Purity | Purity | RF | RRT | Ratio | S/N | Sample | Sample Concentration | Similarity | Synonyms | Synonyms List | Weight |
Library Hits

- Export Library Hits as part of the information for each peak.

Number of library hits to export:

10

Information not exported

- Exact Mass
- Mass Defect
- Sample

Exported Information

- Similarity
- Reverse
- Probability
- CAS
- Library Id
- Formula
- Weight
- Contributor
- Synonyms List

Spectra—

- Export the peak true spectrum as part of the information for each peak.

Mass Threshold (Relative abundance of base ion [0-998])
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