Analysis of Aircraft Cabin Air by TD-GCxGC-TOFMS

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Key Words: Thermal Desorption, SBSE, GCxGC

1. Introduction

Two samples of ambient cabin air from a commercial airliner were collected by Stir Bar Sorption Extraction (SBSE) and analyzed by Thermal Desorption GCxGC-TOFMS. The cabin air is a mixture of re-circulated cabin air and bleed air from the compressor stages of the aircraft's turbine engines. Volatile organic compounds in cabin air, tricresyl phosphate in particular, have been the subject of recent discussion in the media.

2. Instruments and Methods

In this study, measurements were made with a LECO Pegasus 4D GCxGC-TOFMS system. The primary analytical column was 10.0 m x 0.18 mm ID x 0.18 µm df DB-5. The secondary column was 1.00 m x 0.10 mm ID x 0.10 µm df Rxi-17. The temperature program started at 30°C with a 3 minute hold, and then ramped at 5°C/minute to 295°C with a final hold of 3 minutes. The column offset was +10°C with a +15°C modulator offset. A 5.0 second modulation period with a 0.8 second hot pulse was also utilized. Data was acquired over a range of 40 to 400 m/z at 200 spectra/second. Helium was used as the carrier gas at a constant flow of 1.2 mL/minute. The inlet consisted of a GERSTEL Twister Desorption Unit (TDU) connected in-series with a GERSTEL CIS4 inlet. Each sample was collected on a pair of 10 mm x 1.0 mm df PDMS GERSTEL Twister stir bars suspended from a wire scaffold in a 20 mL scintillation vial, as shown in Figure 1. Both stir bars were desorbed simultaneously in Solvent Vent mode at 300°C for 2 minutes and 50 mL/minute flow. The CIS4 was held at -120°C. The injection from the CIS4 to the column was Splitless at 300°C and at column flow.

Figure 1: The sampling apparatus consisting of two PDMS Twister stir bars suspended from a wire scaffold inside of a 20 mL scintillation vial.

Samples were collected during a commercial flight in the business class cabin. Both samples were collected while the aircraft was at cruising altitude and prior to any beverage or food service. The "Active" sample was collected by placing the vial containing the sampling apparatus ~ 8 cm from the overhead air vent operating at maximum flow for a period of 30 seconds. The "Passive" sample was collected by placing the vial containing the sampling apparatus on the open seat-back tray table for a period of 30 minutes. The scintillation vials containing the collected samples were tightly capped and stored immediately following collection.

3. Results

Both of the samples were data processed with a s/n ratio threshold of greater than or equal to 100:1 or 1000:1. A contour plot of the "Active" sample is shown in Figure 2 (A). A contour plot of the "Passive" sample is shown in Figure 2 (B). More detailed plots with peak markers are shown in Figure 3 (Active) and Figure 4 (Passive).

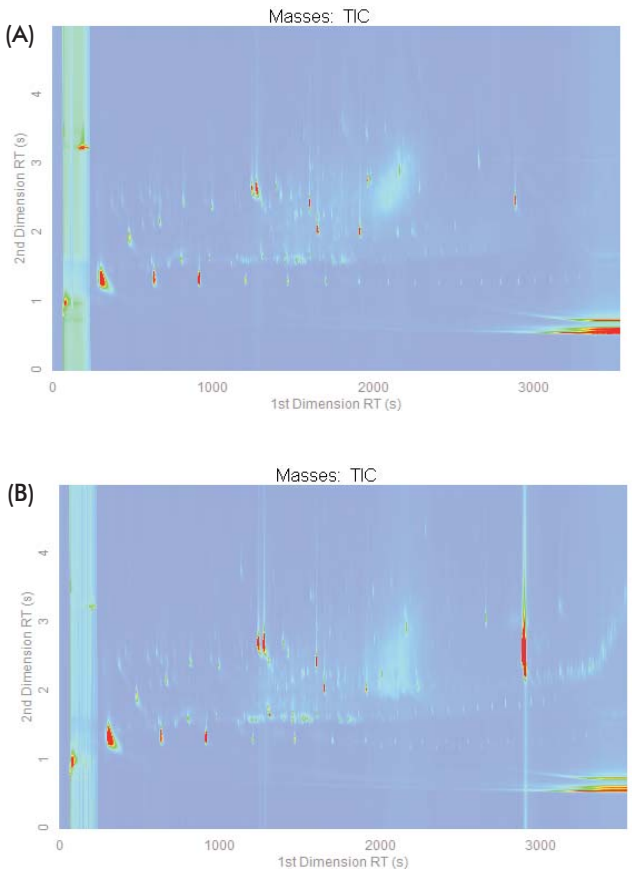

Figure 2: A contour plot of the "Active" sample is shown in (A). A contour plot of the "Passive" sample is shown in (B). The x-axis represents the retention time on the primary column. The y-axis represents the retention time on the secondary column.

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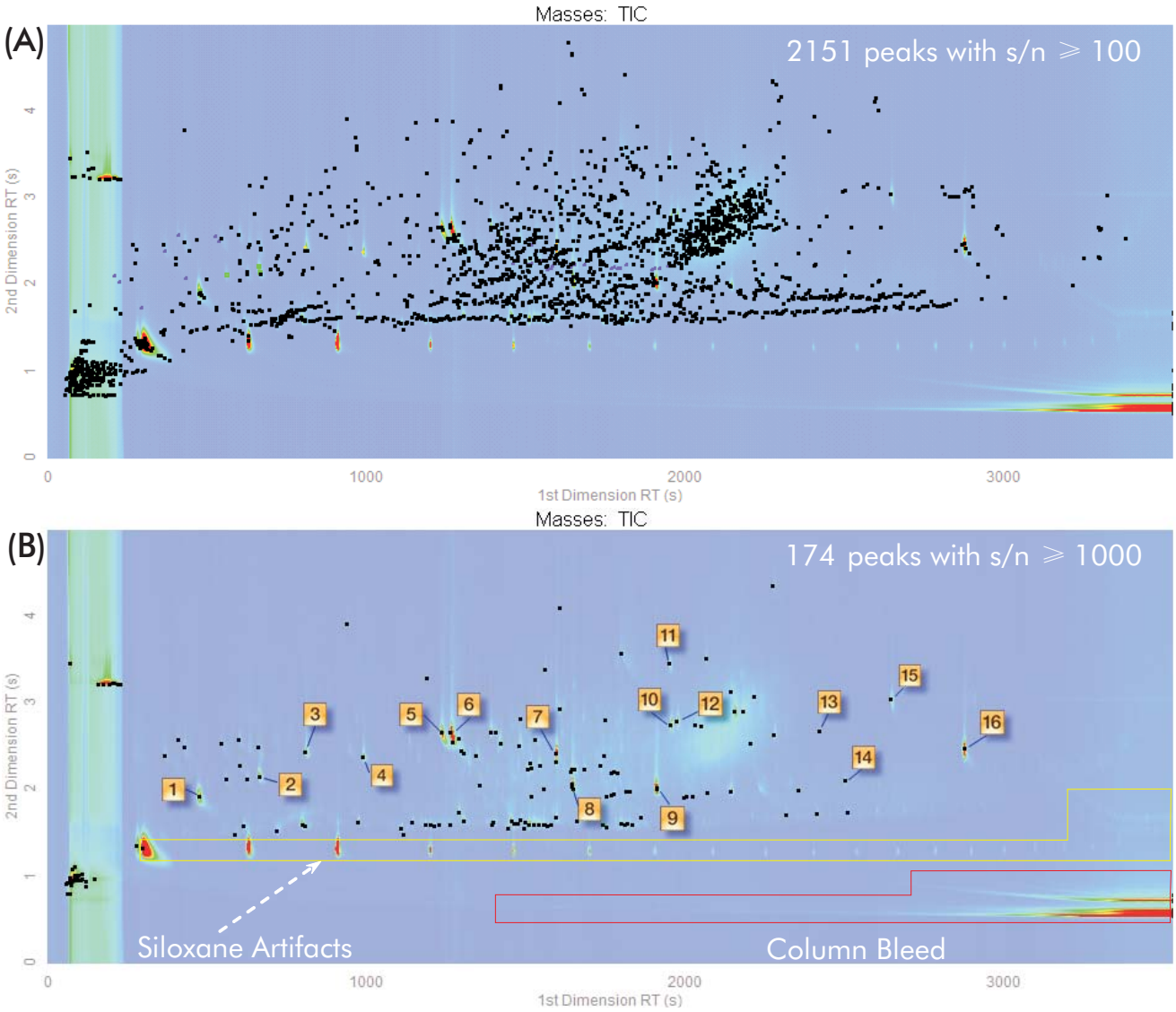

Figure 3: Contour plots of the "Active" sample with Peak Markers. An "Exclusion" Classification Region was used to eliminate peaks resulting from column bleed and siloxane artifacts located along the lower portion of the contour plot. Using a s/n ratio threshold of ⩾100:1(A), 2151 peak were found; a threshold of ⩾ 1000:1(B) returned 174 peaks. Identifications of selected major peaks from (B) are shown in Table 1.

Table 1: ID's of 16 selected major components as indicated in Figure 3 (B).

#	Identification (NIST08 Library similarity out of 1000)	#	Identification (NIST08 Library similarity out of 1000)
1	α-pinene **(926)**	**9**	2-methyl-2-heptanol **(826)**
2	limonene **(933)**	**10**	3,7,11-trimethyl-1,6,10-dodecatrien-3-ol **(792)**
3	nonanal **(932)**	**11**	1,2-benzenedicarboxylic acid, bis(2-methylpropyl) ester **(915)**
4	decanal **(921)**	**12**	3,7,11-trimethyl-2,6,10-dodecatrien-1-ol **(787)**
5	propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl)propyl ester **(891)**	**13**	benzoic acid, undecyl ester **(808)**
6	propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester **(909)**	**14**	hexadecanoic acid, 1,1-dimethylethyl ester **(809)**
7	propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester **(855)**	**15**	1,2-benzenedicarboxylic acid, diisooctyl ester **(905)**
8	2-hexanol, 2,3-dimethyl- **(825)**	**16**	(Z)-2,6,10-trimethyl-1,5,9-undecatriene **(852)**

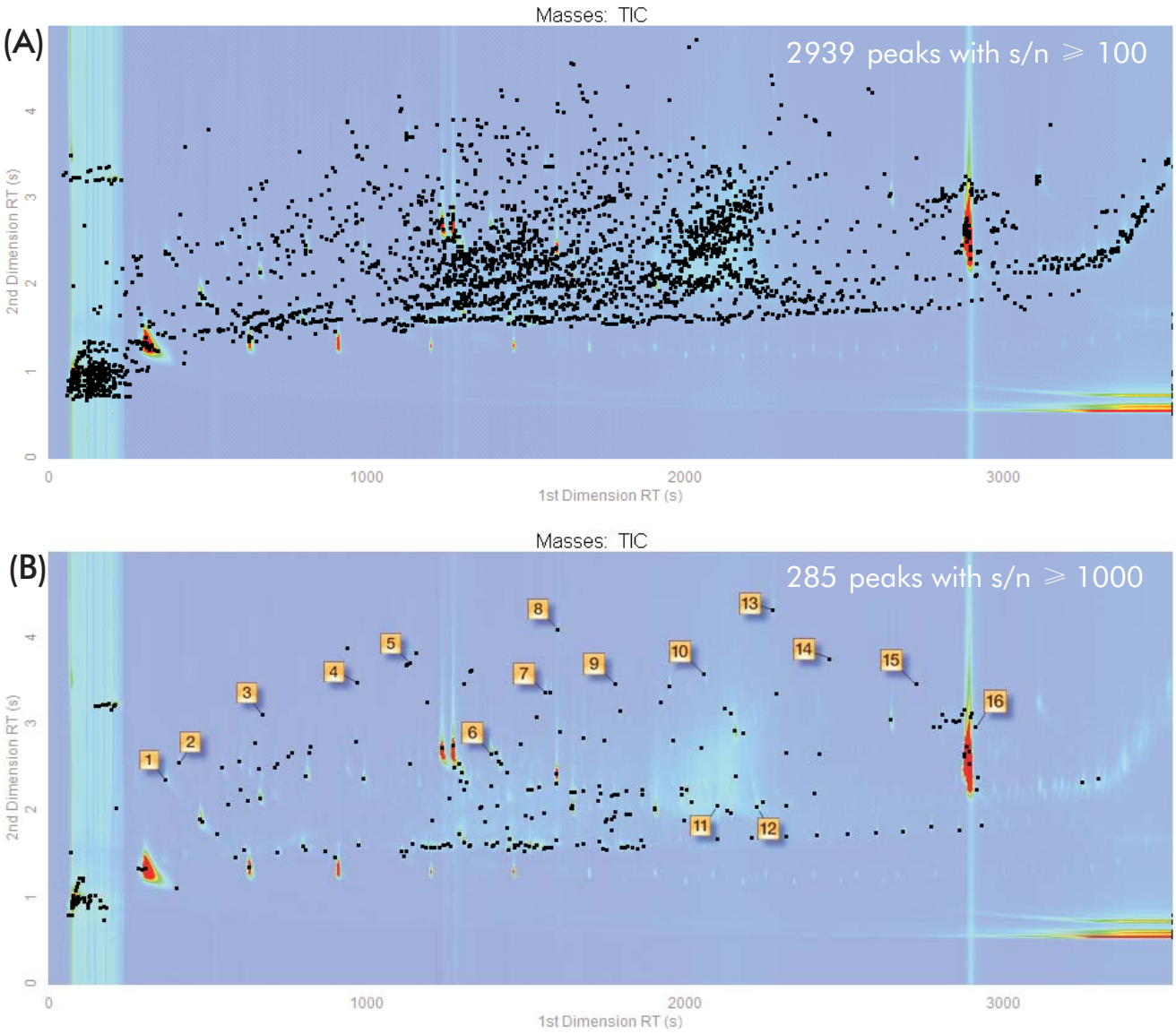

Figure 4: Contour plots of the "Passive" sample with Peak Markers. An "Exclusion" Classification Region was used to eliminate peaks resulting from column bleed and siloxane artifacts located along the lower portion of the contour plot. Using a s/n ratio threshold of ⩾100:1(A), 2939 peaks were found, and a threshold of ⩾ 1000:1(B), returned 285 peaks. Identifications of selected major peaks from (B) not already identified in Table 1 are shown in Table 2.

Table 2: ID's of 16 selected major components as indicated in Figure 4 (B).

#	**Identification** (NIST08 Library similarity out of 1000)	#	**Identification** (NIST08 Library similarity out of 1000)
1	p-xylene **(961)**	**9**	2,6-bis(1,1-dimethylethyl)-1,4-benzenediol **(824)**
2	o-xylene **(953)**	**10**	dibutyl phthalate **(949)**
3	indane **(925)**	**11**	hexadecanoic acid, ethyl ester **(894)**
4	2-hydroxybenzoic acid, methyl ester **(948)**	**12**	trans-9-hexadecen-1-ol **(927)**
5	1-methyl napthalene **(935)**	**13**	diphenylpropanetrione **(955)**
6	(E)-6,10-dimethyl-5,9-undecadien-2-one **(961)**	**14**	1-phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1à,4aá,10aà)]- **(858)**
7	benzoyl isothiocyanate **(836)**	**15**	phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)- **(826)**
8	diethyl phthalate **(956)**	**16**	cholesta-3,5-diene **(881)**

Delivering the Right Results

Selected major components for the Active sample are shown in Table 1. Selected major components for the Passive sample, which were not already identified in Table 1, are shown in Table 2. Tricresyl phosphate is an organophosphate that is a known neurotoxin that is present in the oil used in aviation turbine engines. Tricresyl phosphate was not found in either sample.

Both samples had similar composition, with the propanoic acid esters being a dominant feature. Figure 5 shows the region containing the propanoic acid esters for both samples. These two peaks are identified as peaks 5 and 6 in Figure 3.

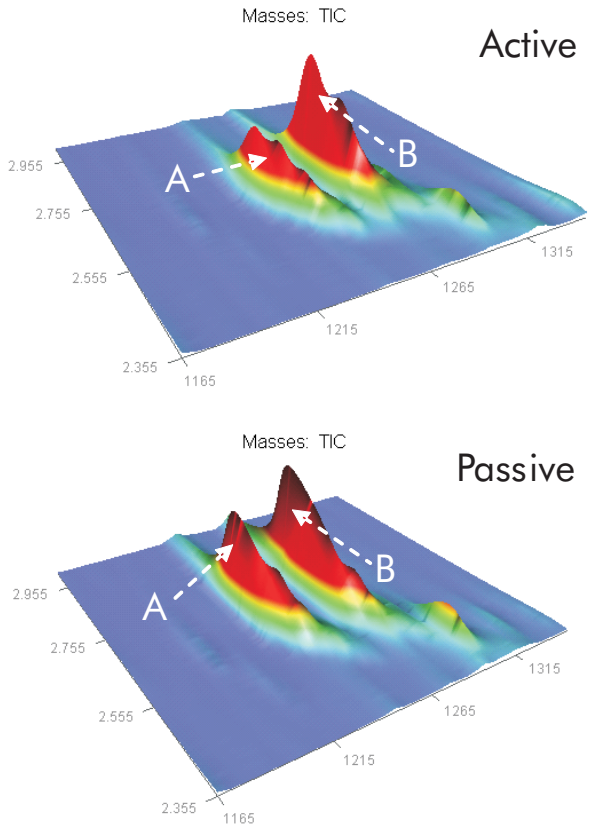

Figure 5: Surface plots of the "Active" and "Passive" samples with the peaks for (A) Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(2-hydroxy-1-methylethyl) propyl ester and (B) Propanoic acid, 2-methyl-,1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester indicated.

In the Passive sample, the very large feature at approximately 2875 seconds is composed of high molecular weight polyunsaturated hydrocarbons, some of which have been hydrolyzed.

4. Conclusions

The recent global outbreaks of SARS, influenza and other highly contagious conditions have led commercial aircraft manufacturers and operators to equip aircraft ventilation systems with HEPA particle filtration. While HEPA filtration does provide a level of protection against particulate pathogens, it does not provide protection from chemical vapors present in the aircraft cabin and ventilation systems. The work presented here provides an example of a simple sampling technique for VOCs and SVOCs in a commercial aircraft cabin. These samples are complex and contain components over a wide range of volatilities and functionalities. When analyzed by GCxGC-TOFMS, the large number of individual components can be resolved and identified in a single analysis, providing an efficient means for the analyst to obtain a large amount of information about the sample with a minimum amount of effort. LECO's Pegasus 4D GCxGC-TOFMS system and ChromaTOF software are an excellent choice for the analysis of highly complex samples such as those demonstrated in this work.

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