Application Note

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A Chemometric Approach for Ambient Air Monitoring Using Thermal Desorption GC/MS

Monitoring VOCs in air using diffusive and active sampling techniques per IS 5182-27 and IS 5182-28

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Abstract

The introduction of National Standard methods IS 5182 Part 27 and Part 28 marks a significant advancement in India's air quality management, providing standardized methodologies for passive and active sampling of volatile organic compounds (VOCs) and semivolatile organic compounds (SVOCs). These pollutants, which come from industrial, vehicular, and urban sources, contribute to secondary aerosol formation and ground-level ozone, exacerbating air pollution. The adoption of thermal desorption gas chromatography/single quadrupole mass spectrometry (TD GC/MS) in these Bureau of Indian Standards (BIS) regulations ensures highly sensitive, accurate, and reproducible detection of hazardous air toxics. This application note describes a TD GC/MS method for analyzing environmental VOCs that is compatible with the BIS regulations and uses an Agilent 8890 GC system with an Agilent 5977C GC/MSD. Data extraction and statistical analysis were performed using Agilent Mass Profiler Professional software. The characteristic VOCs, which were identified or tentatively identified by comparing mass spectra with the U.S. National Institute of Standards and Technology (NIST) library, were subjected to principal component analysis (PCA) and hierarchical clustering analysis to reveal differences among samples collected at different locations and times.

Introduction

Monitoring VOCs is crucial for assessing air quality in industrial and urban settings. These compounds, which include propene, hexachlorobutadiene, and naphthalene, vary in volatility and encompass both polar and nonpolar chemicals. Recognizing the importance of standardized monitoring, the Bureau of Indian Standards (BIS) has developed specific methodologies for these compounds under the IS 5182 series.

IS 5182-27 focuses on the measurement of vapor-phase organic chemicals such as vinyl chloride and nC22 hydrocarbons in air and gaseous emissions. This method employs diffusive (passive) sampling onto sorbent tubes or cartridges, followed by TD (see Figure 1) and capillary GC analysis. The passive sampling approach offers advantages in terms of ease of deployment and cost-effectiveness, making it suitable for widespread monitoring applications.

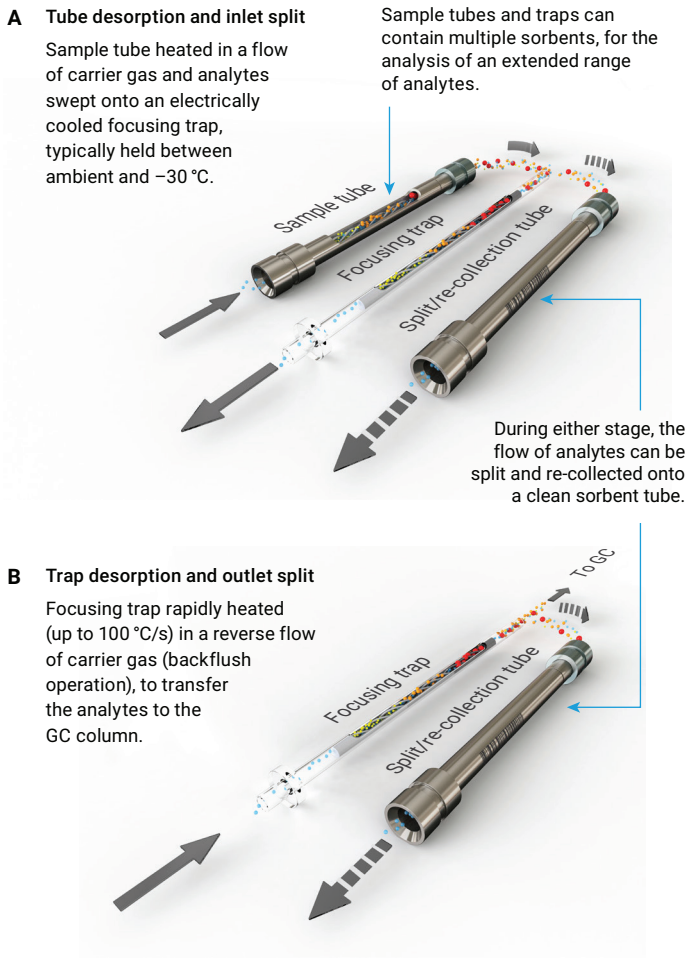

Figure 1. How two-stage thermal desorption works.

IS 5182-28 addresses the measurement of vapor-phase organic chemicals ranging from C3 to nC30 hydrocarbons in air and gaseous emissions. This method involves active sampling, where the sample atmosphere is pumped onto sorbent tubes. These tubes are then sealed and transported to the laboratory for analysis via TD and capillary GC. Active sampling allows for precise control over sample volumes and is particularly useful when dealing with low-concentration pollutants or when shorter sampling durations are required.

The use of sorbent tubes in both methods offer numerous benefits for air monitoring. They are compact, easy to transport, and cost-effective compared to alternatives such as canisters. Sorbent tubes are compatible with a wide range of compounds and sample volumes. Moreover, the TD process used during analysis effectively removes contaminants, allowing the tubes to be reused immediately. In this context, IS 5182-27 uses single sorbent tubes for passive sampling, while IS 5182-28 employs multibed tubes packed with a combination of porous polymer, graphitized carbon black, and carbonized molecular sieves for active sampling. These tailored approaches ensure efficient capture and accurate analysis of a broad spectrum of VOCs, thereby enhancing the reliability of air quality assessments in various environments.

To reveal relevant patterns and sources of variation in these large environmental datasets according to the IS-5182 guidance, this application note proposes chemometric analysis using the Markes TD100-xr automated thermal desorber (Figure 2) and the Agilent 8890 GC system with 5977C GC/MSD (Figure 3). Chemometrics is a discipline that uses mathematics, statistics, and formal logic to design or select optimal experimental procedures. Chemometric techniques commonly used for clustering are the hierarchical agglomerative cluster analysis and PCA with factor analysis.

Figure 2. The Markes TD100-xr automated thermal desorber.

Figure 3. The Agilent 8890 GC system with 5977C GC/MSD.

Sampling approaches

Active sampling experiment

Clean, conditioned, and capped sorbent tubes (Markes part number IS 5182-28) were used with the Markes ACTI-VOC pump for active sampling, ensuring precise flow control of 20 mL/min with the sampling end facing the air source. To begin sampling, the storage cap was removed and the tube was securely attached to the pump's inlet. The pump was then activated, operating at flow rate of 20 mL/min for a period of 1 hour. After sampling, the pump was stopped, the sorbent tube removed, and the storage cap replaced to prevent contamination. The tube was then labelled and stored in an airtight container for transport to the laboratory. This exercise was performed at four different locations: an industrial area, a residential area, a traffic area, and a petrol station area.

Passive sampling experiment

Clean, conditioned, and capped sorbent tubes (Markes part number IS 5182-27) were installed at a field station in industrial area and residential area for passive sampling. At the start of sampling, the storage cap at the sampling end of the tube was removed and replaced with a diffusion cap. Sampling was carried out for three different time periods: 24 hours, 1 week, and 2 weeks, during which gaseous VOCs migrated into the air gap inside the tube and adsorbed onto the sorbent. At the end of the sampling period, the diffusion caps were removed from the sample tubes and replaced with the long-term storage caps, ready for transport to the analytical laboratory.

Table 1. Instrument method parameters.

TD	
Instrument	TD100-xr (Markes International)
Focusing Trap	"TO-15/TO-17 Air toxics" (Markes International part number U-T15ATA-2S)
Tube Desorb	300 °C (10 min)
Tube Dry-Purge	50 mL/min for 6 min
Trap Low	25 °C
Trap High	300 °C (3 min)
Trap Heating Rate	40 °C/s
Outlet Split	10 mL/min
Split Ratio	7.7:1
TD Flow Path	150 °C
GC	
Carrier Gas	Helium
Column	Agilent J&W HP-5ms, 60 m, 0.25 mm × 0.25 µm (part number 19091S-436)
Column Flow	1.0 mL/min
Mode	Constant flow
Oven Ramp	40 °C (5 min), 15 °C/min to 300 °C (10 min)
MS	
MS Source	230 °C
MS Quad	150 °C
Scan Range	33 to 500 amu

Results and discussion

Active (pumped) sampling experiment results

The TD GC/MS data analysis using NIST library matching showed interesting results for the active sampling experiment. Agilent Mass Profiler Professional software was used for statistical evaluation of components obtained as various locations. To fully characterize compounds of all the location samples, GC/MS analysis was conducted in duplicates for the industrial, residential, petrol pump, and traffic areas, respectively. This method can clearly differentiate VOC compounds observed at different locations. Table 2, Figure 4, and Figure 5 show the difference in chromatograms, peak intensities, and hierarchy between samples collected from different locations.

Table 2. Details of peaks found in the ambient air at various locations using the active sampling approach.

Compound	Retention Time	Formula	Peak Areas (Counts)			
			Industrial Area	Residential Area	Traffic Area	Petrol Pump Area
Isobutane	4.27	C_4H_{10}	3041320.2	468432.75	9146850	2996008.5
Butane	4.35	C_4H_{10}	3688527	1023541	1.60E+07	5109639.5
Dimethyl ether	4.54	C_2H_6O		121631.27	2991433.2	1003266.56
Butane, 2-methyl-	4.64	C_5H_{12}	1222821.8	781675.4	1.18E+07	4265469
Butane, 2,2-dimethyl-	5.09	C_6H_{14}			7328023.5	
Methylene chloride	5.11	CH_2Cl_2	2192306.8	495920.8		3383261.8
Pentane, 2-methyl-	5.44	C_6H_{14}	1579275.9	422844	6242053.5	2091415
n-Hexane	5.86	C_6H_{14}	2692989		2903597.2	1420466.1
Furan, 3-methyl-	5.96	C_5H_6O			446985.03	
Ethyl Acetate	6.12	$C_4H_8O_2$	4389009.5	4291925.5	2141063	3385758.5
Trichloromethane	6.20	$CHCl_3$			1034087.7	2055782.6
Cyclopentane, methyl-	6.38	C_6H_{12}		65024.945	2041676.4	797134.44
Ethane, 1,2-dichloro-	6.77	$C_2H_4Cl_2$				551735
Benzene	7.01	C_6H_6	3547298.5	1451188.4	8376306.5	5442389.5
Hexane, 3-methyl-	7.21	C_7H_{16}	399943.3		1215171.5	416916.6
2-Heptene, (E)-	7.53	C_7H_{14}			456108.9	
Heptane	7.70	C_7H_{16}	731630.06		1873867.2	474079.88
Propane, 1,2-dichloro-	7.73	$C_3H_6Cl_2$				936610.4
Trichloroethylene	7.75	C_2HCl_3		2071078.4		
Cyclohexane, methyl-	8.25	C_7H_{14}	615195	98841.336	1621972.9	539065.9
Heptane, 2-methyl-	9.06	C_8H_{18}			808422.6	318139.66
Toluene	9.15	C_7H_8	2.00E+07	5163218	2.15E+07	1.55E+07
Heptane, 3-methyl-	9.22	C_8H_{18}			1614181.9	
Cyclohexane, 1,4-dimethyl-	9.38	C_8H_{16}				410847.34
Cyclohexane, 1,3-dimethyl-, cis-	9.38	C_8H_{16}			954842	
Octane	9.75	C_8H_{18}	306968.22	100447.7	1322184.1	525742.1
Tetrachloroethylene	10.02	C_2Cl_4		347420.75	451019.2	
Acetic acid, butyl ester	10.05	$C_6H_{12}O_2$	4518481.5	256097.11	654001.94	1544849
Cyclohexane, ethyl-	10.46	C_8H_{16}			528660.5	
2,4-Dimethyl-1-heptene	10.56	C_9H_{18}				177703.16
Ethyl benzene	10.97	C_8H_{10}	1.47E+07	1269611.1	6040983	4216510
1-Methoxy-2-propyl acetate	11.04	$C_6H_{12}O_3$	1212550.9			573772.5
Benzene, 1,4-dimethyl-	11.11	C_8H_{10}	1.35E+07	1405508.6	1.23E+07	7513198.5
Styrene	11.48	C_8H_8		126308.68	616893.1	455101.8
o-Xylene	11.52	C_8H_{10}	6011600	863551.7	6971842.5	4160620
2-Ethoxyethyl acetate	11.66	$C_6H_{12}O_3$	677679.25			

Compound	Retention Time	Formula	Peak Areas (Counts)			
			Industrial Area	Residential Area	Traffic Area	Petrol Pump Area
Ethanol, 2-butoxy-	11.67	$C_6H_{14}O_2$				245637.9
Benzene, propyl-	12.46	C_9H_{12}	623009.1	208160.31	1206586	591024.8
Tridecane, 6-methyl-	12.51	$C_{14}H_{30}$	199965.58			
Mesitylene	12.84	C_9H_{12}		610122.1	1134736.5	
Cyclotetrasiloxane, octamethyl-	12.86	$C_8H_{24}O_4Si_4$		435862.28		
Heptane, 2,2,4,6,6-pentamethyl-	12.94	$C_{12}H_{26}$	590687.4			
Benzene, 1,2,4-trimethyl-	13.02	C_9H_{12}	4651158		5874188.5	2395739.2
Octanal	13.07	$C_8H_{16}O$		151189.2		
Benzene, 1,2,3-trimethyl-	13.24	C_9H_{12}	1207457.4	193015	1851607.5	693057.06
Eucalyptol	13.55	$C_{10}H_{18}O$			340272.56	
Indane	13.64	C_9H_{10}	249583.81	104745.79	918558.1	230808.62
2-Indanol	13.76	$C_9H_{10}O$			1397234.4	519186.47
Benzene, 2-ethyl-1,4-dimethyl-	13.84	$C_{10}H_{14}$	676193.6		1247937.2	437732.75
3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	14.08	$C_{10}H_{14}$			3056638	
Undecane	14.22	$C_{11}H_{24}$	913803.94	241886.73	1379415.9	609851.2
Linalool	14.27	$C_{10}H_{18}O$			414321.4	
4,7-Methano-1H-indene, octahydro-	14.42	$C_{10}H_{16}$		90211.12	711840.5	
2-Naphthalenol, decahydro-	14.42	$C_{10}H_{18}O$				186096.03
Benzene, 1,2,3,4-tetramethyl-	14.62	$C_{10}H_{14}$	763600		552894.56	
Tricyclo[5.2.1.0(2,6)]dec-4-ene, 4-methyl-	14.95	$C_{11}H_{16}$			770811.6	
Cyclohexanol, 5-methyl-2-(1-methylethyl)-	15.19	$C_{10}H_{20}O$			342878.22	
Dodecane	15.31	$C_{12}H_{26}$	707173.9	214410.81	1051042.4	527086.75
1H-Indene, 2,3-dihydro-1,6-dimethyl-	15.38	$C_{11}H_{14}$			183315.19	
Tridecane	16.30	$C_{13}H_{28}$	490031	99801.47	528903.75	444505.22
Hexadecane, 2,6,10,14-tetramethyl-	17.03	$C_{20}H_{42}$	134408.11			
Tetradecane	17.22	$C_{14}H_{30}$	1149604.1	112018.125	582559.6	937837.06
Pentadecane	18.08	$C_{15}H_{32}$	385732.06		298211.8	360338.66
Diethyl Phthalate	19.01	$C_{12}H_{14}O_4$			309645.75	161226.88
[1,1':3',1"-Terphenyl]-2'-ol	23.63	$C_{18}H_{14}O$	240288.61			164286.81

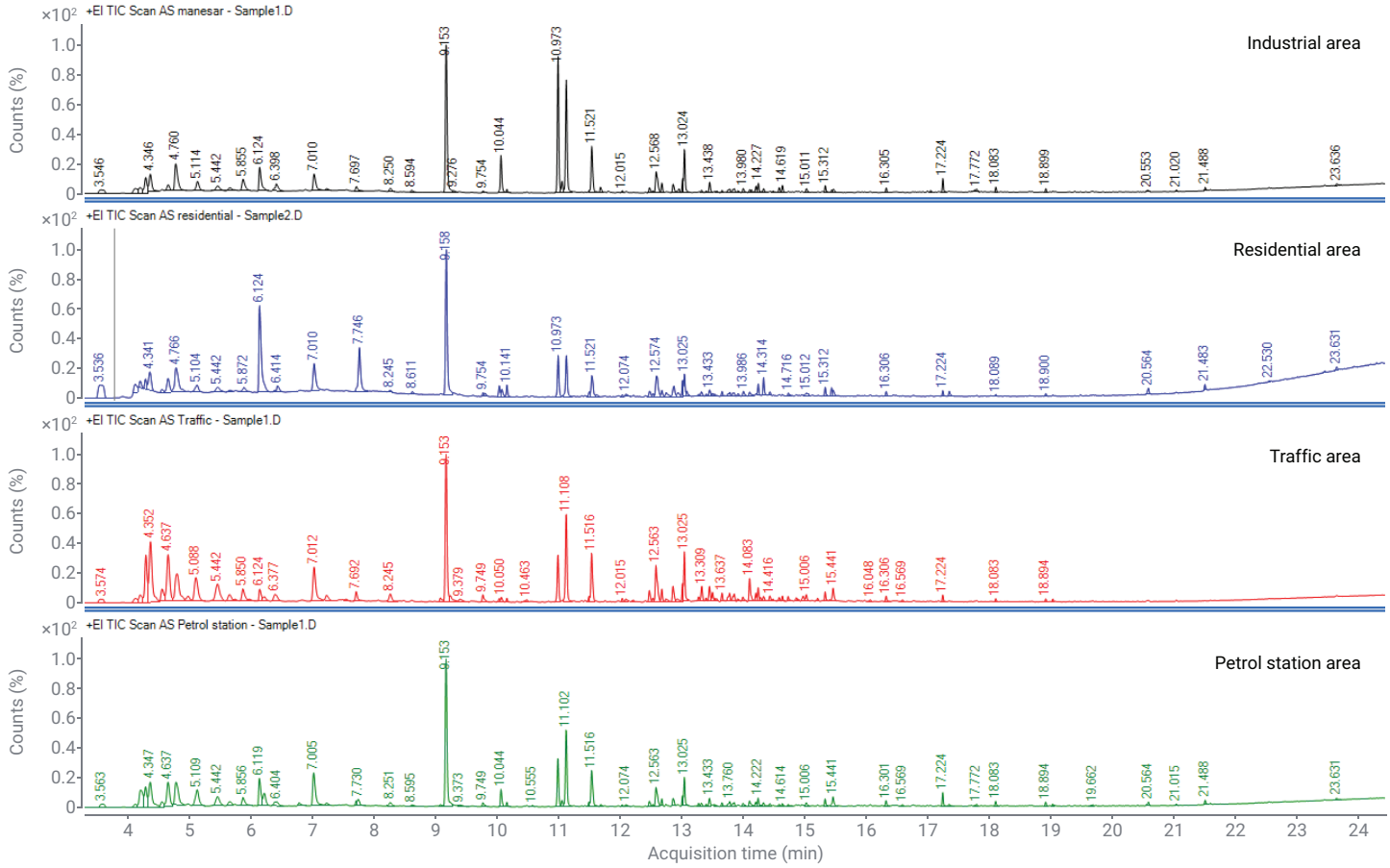

Figure 4. Chromatograms obtained from active sampling experiments at four different locations: an industrial area, a residential area, a traffic area, and a petrol station area.

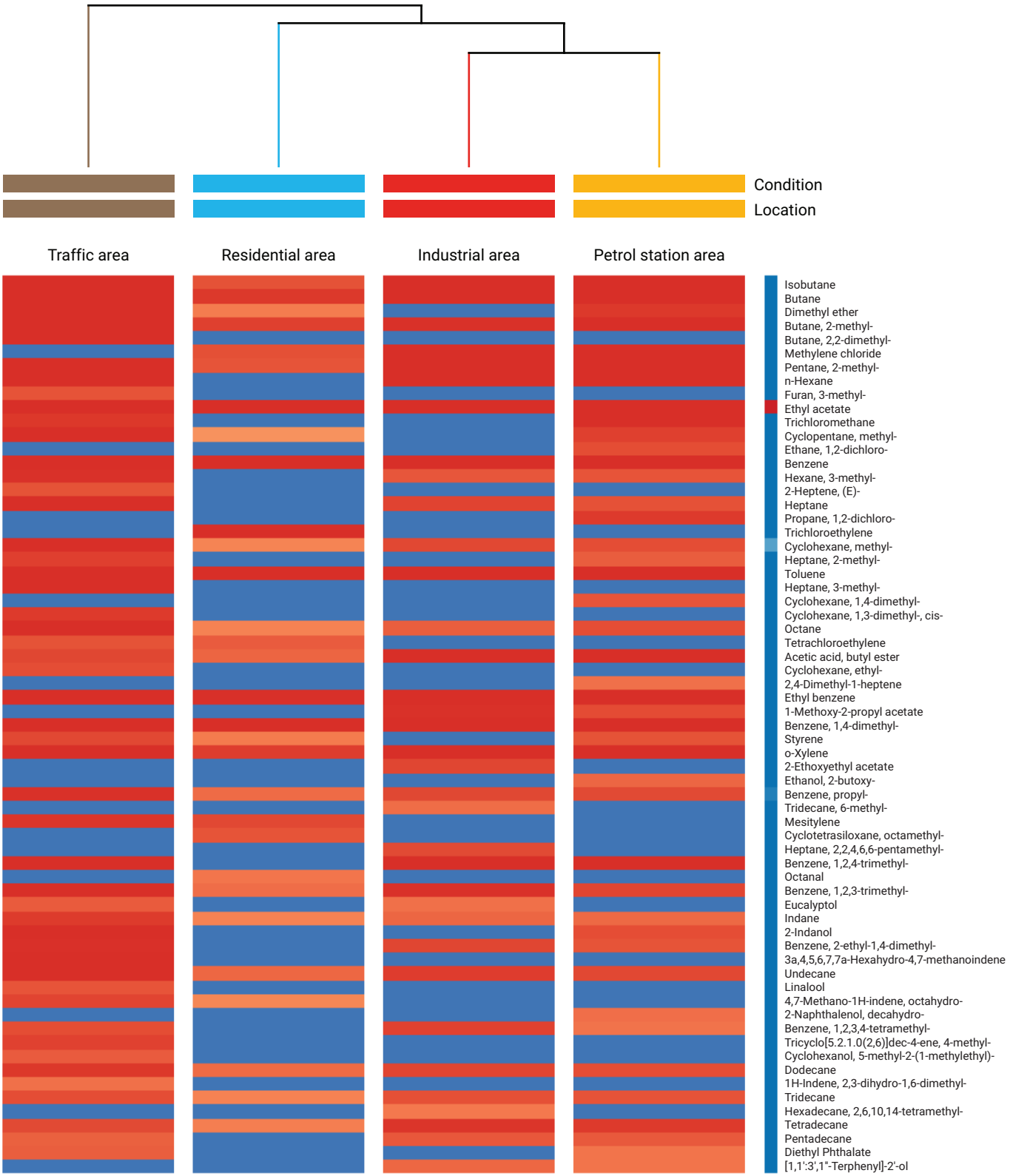

Figure 5. Hierarchical cluster analysis plot for compounds found at all four locations.

Figure 6 shows a Venn diagram identifying the similar and different entities all together from sampling in different areas. The figure indicates that the sampling near the traffic and petrol areas had a higher number of relevant potential VOC compounds. Table 3 shows the list of unique compounds found at each location.

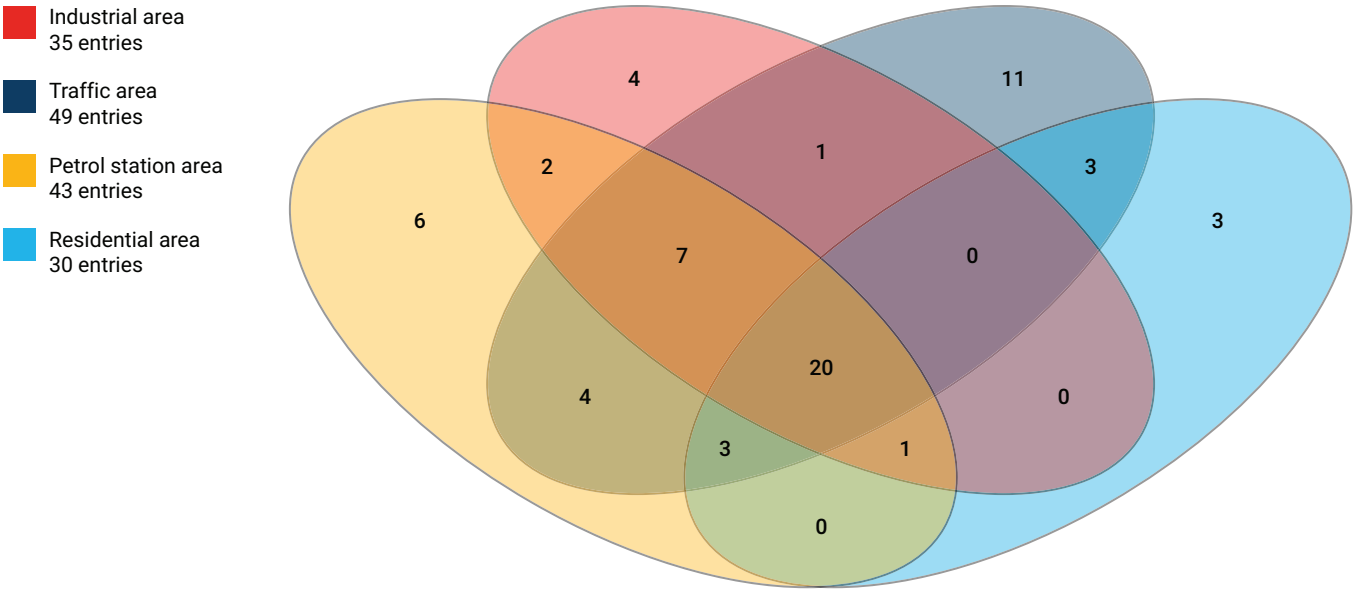

Figure 6. A Venn diagram shows the number of unique and common compounds found in ambient air at four different locations.

Table 3. Unique peaks found in ambient air at each sampling location.

Industrial Area	Petrol Pump Area	Traffic Area	Residential Area
Heptane, 2,2,4,6,6-pentamethyl-	Cyclohexane, 1,4-dimethyl-	Tricyclo[5.2.1.0(2,6)]dec-4-ene, 4-methyl-	Trichloroethylene
Hexadecane, 2,6,10,14-tetramethyl-	2-Naphthalenol, decahydro-	2-Heptene, (E)-	
2-Ethoxyethyl acetate	2,4-Dimethyl-1-heptene	Heptane, 3-methyl-	Octanal
Tridecane, 6-methyl-	Propane, 1,2-dichloro-	3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	
	Ethanol, 2-butoxy-	Linalool	
	Ethane, 1,2-dichloro-	Furan, 3-methyl-	
		Butane, 2,2-dimethyl-	
		Cyclohexane, 1,3-dimethyl-, *cis*-	
		Cyclohexanol, 5-methyl-2-(1-methylethyl)-	
		Cyclohexane, ethyl-	
		1H-Indene, 2,3-dihydro-1,6-dimethyl-	

Due to the complexity of GC/MS-based data comprising the qualitative and quantitative discrepancies of various compounds, multivariate analysis was applied using PCA (Figure 7). All samples and their replicates from each location were constructed and then subjected to this multivariate analysis.

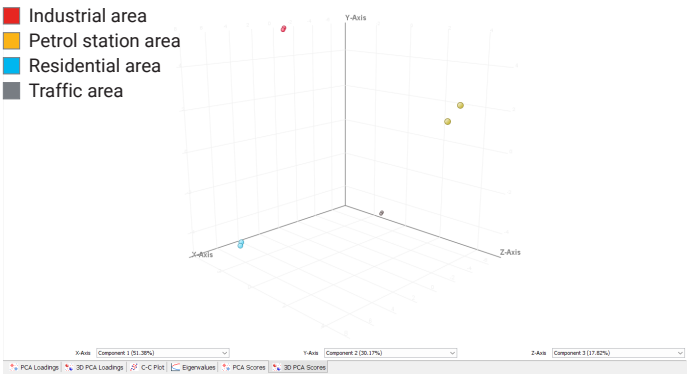

Figure 7. A PCA plot of the active sampling experiment shows the distribution among various samples

Passive (diffusion) sampling experiment results

The TD GC/MS data analysis using NIST library matching showed interesting results for the passive sampling experiment. Figure 8 shows the overlays of chromatograms obtained from sampling for different time durations. A clear increase in peak intensities between 24-hour sampling and 1-week sampling data was observed, whereas between 1-week and 2-week sampling, there was no major rise in peak intensities. This was also confirmed with the peak intensities, as shown in Table 4, which indicates that 1-week sampling gave sufficient uptake of analytes onto sorbent tubes. Agilent Mass Profiler Professional software was used for statistical evaluation of components obtained for each dataset.

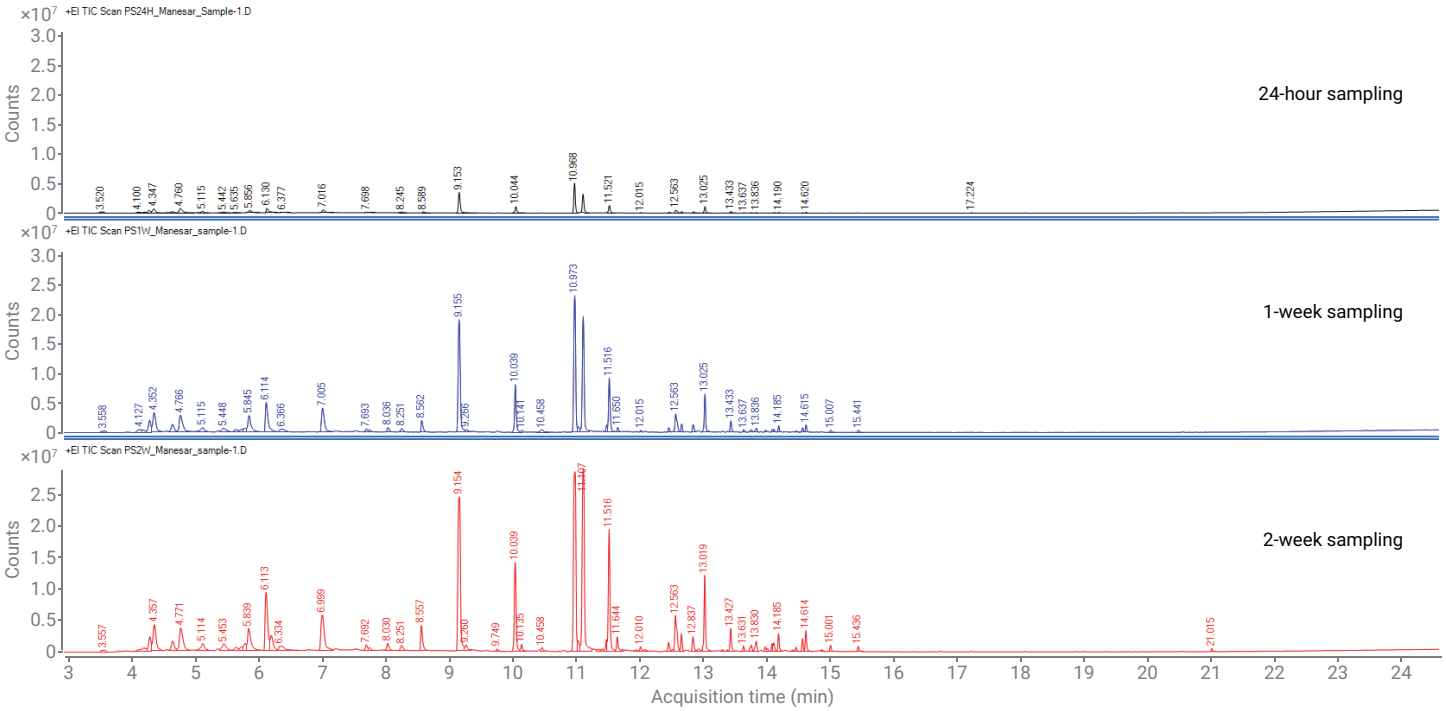

Figure 8. Chromatogram overlays for passive sampling at an industrial area for sampling periods of 24 hours, 1 week, and 2 weeks, respectively.

Table 4. Details of peaks found in ambient air at two locations using the passive sampling approach.

Compound	Retention Time	Industrial Area Peak Intensities			Residential Area Peak Intensities		
		24-Hour Sampling	1-Week Sampling	2-Week Sampling	24-Hour Sampling	1-Week Sampling	2-Week Sampling
Isobutane	4.26	1362105	5656029	6366694	2306082	5068887	5782100
Butane	4.33	2417938	11835481	15338583	4000635	11470533	12845179
Dimethyl ether	4.52	212842			336057		
Butane, 2-methyl-	4.62	791684	3423134	5455864	1323390	5009245	5309458
Oxirane, trimethyl-	4.75	3265432		14236564	5027953	6912901	7116943
Acetone	4.76		10249169				
Methylene chloride	5.09	859704	3076771	5018183	1432952	7707831	6824494
Pentane, 2-methyl-	5.42	588106	3486643	4071046	541446	4218726	6809033
Pentane, 3-methyl-	5.62	267529	1787971	1967717		1460580	2483818
Methyl vinyl ketone	5.72			1474468			
Methoxyacetic acid, pentyl ester	5.73		1491220				
Ethanamine, 2-propoxy-	5.75					3039295	
Butanal	5.78			3374045			
2-Pentanone, 3-methyl-	5.82	1668982			624514	7230448	11183679
2-Butanone	5.84		12311634	13336744			
Furan, 3-methyl-	5.91						820634
Ethyl Acetate	6.1	2068814	15128358	25819750	2783787	17934704	28107654
Trichloromethane	6.16				1435580		
1,3,5-Trifluorobenzene	6.19			5458611			
1-Propanol, 2-methyl-	6.33			3825585			
Cyclopentane, methyl-	6.34	248133	2682123		221891	1720650	3892655
Tetrahydrofuran	6.4	314825					
Ammonium acetate	6.45						1734972
Benzene	6.98	1881690	13225938		2627605	12931736	22949696
Pentane, 2-chloro-2-methyl-	6.99			20659238			
Hexane, 3-methyl-	7.16					1039162	1760738
Heptane	7.67	182705	1061730	1838357	336416	1511206	1934766
Trichloroethylene	7.72	233860	958630	1178230	223645	1101447	1866266
n-Propyl acetate	8.03		1865414	2875781			
Cyclohexane, methyl-	8.22	454016	1693821	2441263	213869	1552447	2108248
Methyl Isobutyl Ketone	8.56	422780	4347334	8916293	143988		762133
Heptane, 2-methyl-	9.02						690063
Toluene	9.13	7211756	45562748	69322944	8792872	41945472	56941536
Isobutyl acetate	9.26		1352496	3108707			
Cyclohexane, 1,3-dimethyl-, cis-	9.34						1474852
Octane	9.72			813344	81153	864693	1301258
Tetrachloroethylene	9.98				71866		
Acetic acid, butyl ester	10	2131870	15099847	28226446	679816	2841221	3678187
Cyclotrisiloxane, hexamethyl-	10.1	170873	435966	2980536	820124	414049	1627158
Cyclopentane, propyl-	10.4			621600			
Pyrazole, 1,4-dimethyl-	10.4						1270099
Cyclohexanemethanol, .alpha.-(2-methyl-2-propenyl)-	10.4		1869306			654227	
Cyclohexane, ethyl-	10.4			1516070			
Ethyl benzene	10.9	8512412		79367224	5202252	12877530	15610185
1-Methoxy-2-propyl acetate	11.03		1816770				

Compound	Retention Time	Industrial Area Peak Intensities			Residential Area Peak Intensities		
		24-Hour Sampling	1-Week Sampling	2-Week Sampling	24-Hour Sampling	1-Week Sampling	2-Week Sampling
Benzene, 1,4-dimethyl-	11.08	5734480	40935632	74469736	4102540	14393504	18453732
1-Undecanol	11.34			1271446			
1-Ethyl-4-methylcyclohexane	11.4			1030743			
Styrene	11.45		1724279	3136412	553718	1744349	1900205
o-Xylene	11.5	2458114	16903896	36384432	1988821	7407916	9050857
2-Ethoxyethyl acetate	11.64		1496704	4629116			
Pyrazine, 2,5-dimethyl-	11.77			715707			
2-Propylcyclohexanol	11.94			999845			
Benzene, (1-methylethyl)-	11.99	86126	428693	1462962	101389	474492	427413
Cyclohexane, propyl-	12.07			1161360	119101		
Benzene, propyl-	12.43	254882	1517537	2677187	313313	1355981	1436836
Cyclohexane, 1,1,2,3-tetramethyl-	12.48				97127		
1-Dodecanol, 3,7,11-trimethyl-	12.51			638946			
Benzene, 1-ethyl-4-methyl-	12.59	424594	7927476	14212562	1060425	5538718	6420008
Octanal, 7-hydroxy-3,7-dimethyl-	12.72			986410			
Benzene, 1-ethyl-2-methyl-	12.74	1329220	2638022	4601157			
Cyclotetrasiloxane, octamethyl-	12.83				644405		
Benzonitrile	12.88					617214	734085
Heptane, 2,2,4,6,6-pentamethyl-	12.93			1318103			
Mesitylene	13			20163016	1754480		
Benzene, 1,2,3-trimethyl-	13.01	1905053	11220077	6081778	252660	4596248	4954607
Benzene, 1,2-dichloro-	13.28		397772		89861	1089216	934745
Indane	13.615	81248	690096	1273513	177677	849993	652948
Benzene, 1-methyl-4-propyl-	13.755		1070408	2076652			
Benzene, 2-ethyl-1,4-dimethyl-	13.952	195667	1502584	3144568			
Benzene, 1-methyl-2-propyl-	13.975		592257	999587			
Benzaldehyde, 4-methyl-	14.007			763212			
3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	14.05					1361665	712969
o-Cymene	14.109			2183595			
p-Cymene	14.109	89340					
Benzene, 1-ethyl-2,4-dimethyl-	14.1845		1994385	4219690			
Nonanal	14.287				138869		
4,7-Methano-1H-indene, octahydro-	14.378				312588	1159716	746796
Benzene, 1,2,3,5-tetramethyl-	14.598	110711	2273585	4975827			
Benzene, 1,2,4,5-tetramethyl-	14.614	186572					
Cyclopentasiloxane, decamethyl-	14.684				103960		
1H-Indene, 2,3-dihydro-5-methyl-	14.866			404387			
2-(4-Isopropylphenyl)ethanamine	15.0035		777512	1371786			
Dodecane	15.285				90817		
Decanal	15.387				216280		
Naphthalene	15.441		820970	1416110			
Tridecane	16.273				123302		
Cyclohexasiloxane, dodecamethyl-	16.429				88788		
Tetradecane	17.208	103945			213257		
Cycloheptasiloxane, tetradecamethyl-	17.97				115263		
Pentadecane	18.051				159432		

Compound	Retention Time	Industrial Area Peak Intensities			Residential Area Peak Intensities		
		24-Hour Sampling	1-Week Sampling	2-Week Sampling	24-Hour Sampling	1-Week Sampling	2-Week Sampling
Hexadecane	18.867				209434		
Cyclooctasiloxane, hexadecamethyl-	19.334				125823		
Tritriacontane	19.683				100437		
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	20.988				866504		

Figure 9 shows a PCA chart showing the peak distribution obtained in each dataset. The PCA plot shows variations in 24-hour and 2-week sampling. However, 1-week sampling results show consistent replicate results.

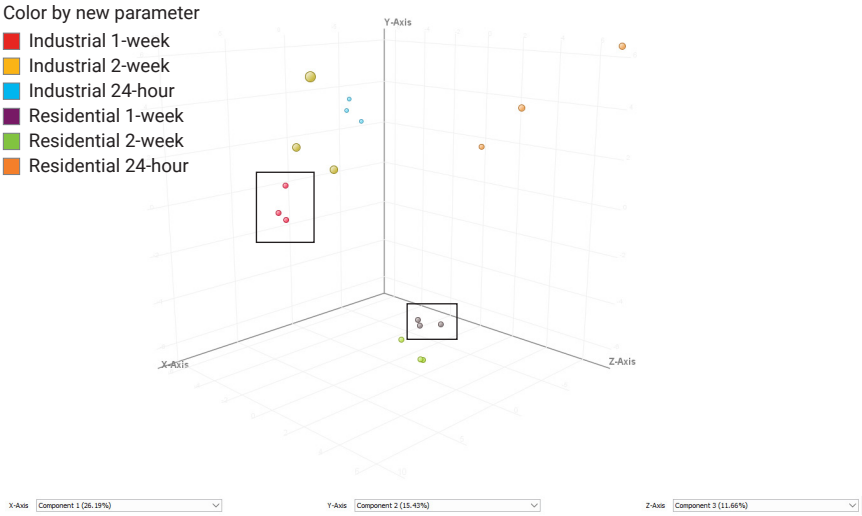

Figure 9. PCA plot of passive sampling experiment to show the distribution among various samples.

BTEX quantitation results

Benzene, toluene, ethyl benzene, and xylenes (BTEX) standards were diluted in methanol and loaded onto the sorbent tubes using a calibration solution loading rig. The resulting concentrations of these standards on the sorbent tubes were 20, 50, 100, 200, and 400 ng, respectively. Figure 10 shows an overlay of these calibration standards.

Figure 11 shows the resulting calibration curves for the BTEX standards. R^2 values of all the calibration curves were above 0.99. This calibration was used to quantify all the samples of active as well as passive sampling experiments. Table 5 shows the resulting concentration in ng/L for BTEX in samples.

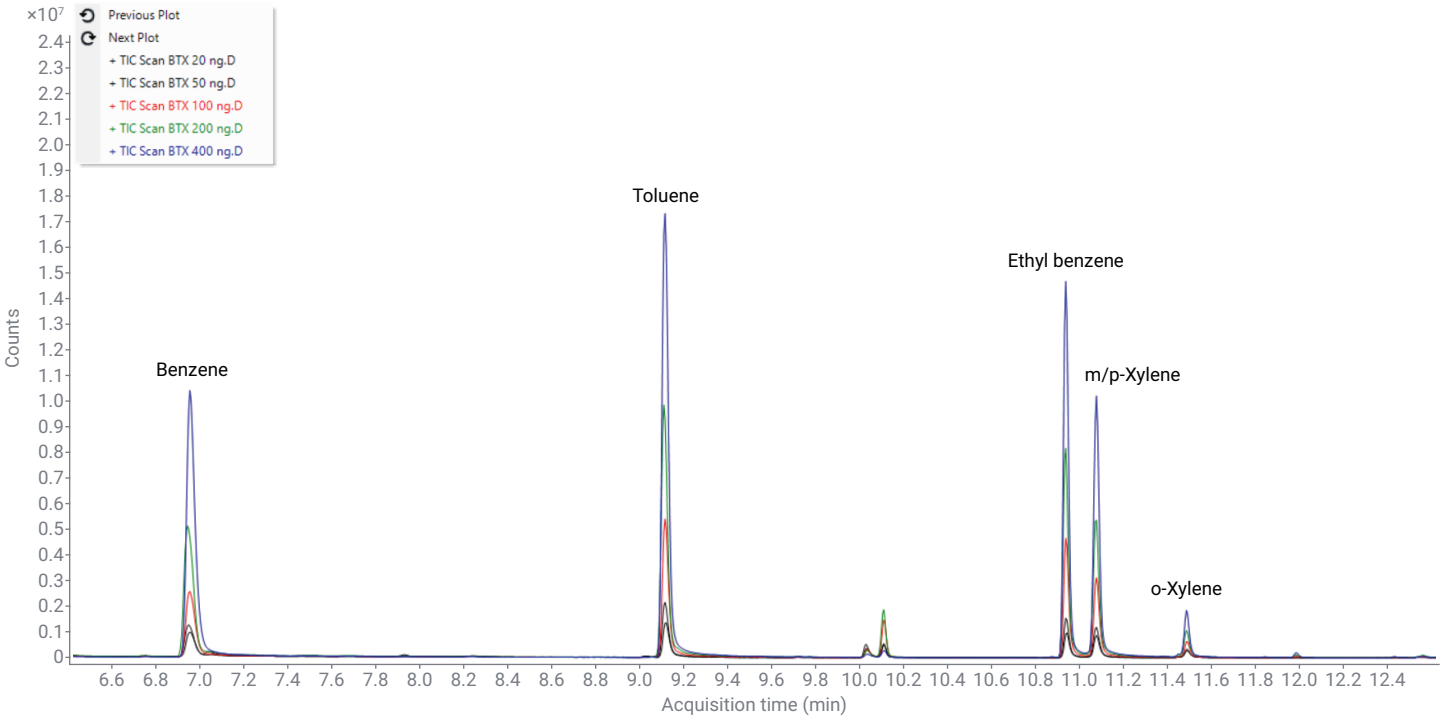

Figure 10. Standard chromatogram overlays of BTEX standards from 20 ng to 400 ng.

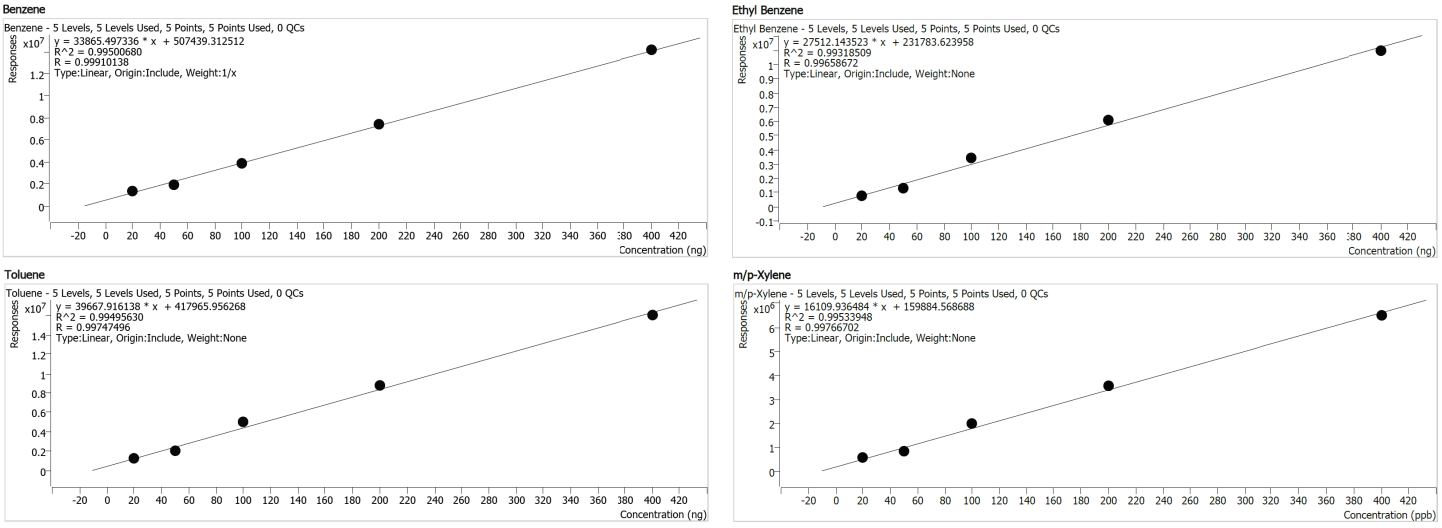

Figure 11. Calibration curves of BTEX standards from 20 ng to 400 ng.

Table 5. Quantification of BTEX standards in active sampling experiments.

Location		Benzene (ng/L)	Toluene (ng/L)	Ethyl Benzene (ng/L)	m/p-Xylene (ng/L)
Industrial Area	Sample 1	4.77	47.28	44.64	54.12
	Sample 2	5.11	48.79	45.94	56.42
Residential Area	Sample 1	4.09	11.88	3.58	5.33
	Sample 2	4.31	13.37	4.06	5.88
Traffic Area	Sample 1	18.64	53.08	18.43	51.15
	Sample 2	18.57	52.60	18.29	51.22
Petrol Station Area	Sample 1	12.06	44.91	16.21	38.71
	Sample 2	8.69	30.66	10.88	25.56

Table 6. Quantification of BTEX standards in passive sampling experiments.

Location (1-Week Sampling)		Benzene (ng/L)	Toluene (ng/L)	Ethyl Benzene (ng/L)	m/p-Xylene (ng/L)
Industrial Area	Sample 1	13.4	80.3	130.9	151.1
	Sample 2	12.6	78.1	127.8	150.7
	Sample 3	12.7	78.6	128.9	148.0
Residential Area	Sample 1	20.0	72.7	37.6	53.6
	Sample 2	19.3	71.6	38.2	54.5
	Sample 3	19.9	71.8	35.5	52.5

Conclusion

This application note highlights the comparison of different air sampling strategies and shows their effect on qualitative and quantitative analysis of VOCs. Active (pumped) sampling helped with faster analysis, which is required for controlled and sensitive real-time monitoring of ambient air. Chromatograms of air sampled at various locations showed the presence of VOCs such as benzene, toluene, ethyl benzene, and xylenes. Many common and unique compounds were found at each location. The intensity of these compounds showed variations at different locations. Fewer compounds with lower intensities were observed in air samples from a residential area, whereas more compounds with higher intensities were observed in air samples from a traffic area. Passive sampling was a comparatively cost-effective and long-term approach and provided consistent replicate results. The chromatographic overlays of different sampling times indicated an increasing trend in peak intensities with respect to time. There was a considerable rise in peak intensities for the 1-week sampling period, as compared to 24-hour sampling. There was a slight rise in peak intensities for the 2-week sampling period, as compared to 1-week sampling. The PCA plot suggested the peak distribution obtained in each dataset. One-week sampling results showed consistent replicate results. Use of the chemometrics software Agilent Mass Profiler Professional added value by providing data visualization for interpretation.

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