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Profiling of volatile organic compounds for environment discrimination in Vilnius City

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The aim of this study was to show how volatile organic compounds (VOCs) profiling can be used as a method to identify different environments across a city. To achieve that, we employed several methods. First, we carried out the profiling of VOCs in several different locations. Then we identified the marker compounds and their sources. Air samples were collected from 6 different locations within the Vilnius City centre using thermal desorption (TD) tubes. Samples were analysed using thermal desorption coupled with gas chromatography mass spectroscopy (TD/GC-MS) methodology. Compound identification was performed by the library match using the NIST MS Search 2.0 (2005) mass spectral library. The results show how variation in the levels of different VOCs can distinguish between locations within a relatively small area of 2 km^2 depending on different emission sources.

Keywords: VOC, thermal desorption, chromatography, anthropogenic, biogenic

INTRODUCTION

Volatile organic compounds (VOCs) are compounds with a high vapour pressure and a low solubility in water. Any organic compound having an initial boiling point less than or equal to 250°C measured at a standard atmospheric pressure of 101.3 kPa is considered a VOC [1]. Thousands of VOCs have been identified from a wide range of sources [2, 3]. VOCs are precursors of O_3 and secondary organic aerosols (SOAs). Therefore, those compounds significantly contribute to the formation of photochemical smog, atmospheric oxidative capacity, visibility degradation and global climate changes [4–6].

VOCs can be biogenic and anthropogenic. Terrestrial vegetation is the dominant source of atmospheric VOCs accounting for about 90% of the total emission globally [7]. Isoprene and monoterpenes are the most abundant species among the biogenic VOCs [8]. Both isoprene and monoterpenes are mainly emitted in the tropical region (88 and 83 % of the global total, resp.). Nevertheless, aromatic hydrocarbons are the most common VOCs to which we are exposed everyday in urban locations. Those VOCs are produced in human activities (anthropogenic source), mainly from fossil fuel emissions and they are considered cancerogenic [9]. As those compounds are a concern for human health their levels are one of the main parameters when considering environmental contamination, together with particle matter, CO_2, ozone and nitrogen oxide [10].

Both types of VOCs contribute to causing climate change and can be cancerogenic. Therefore, in recent years, much research has focused on the impacts of VOCs due to their influence on atmospheric chemistry and impacts on human health [11–13]. Consequently, VOCs profiling is widely used in many environments as an indicator

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for air quality. Most of the studies that analyse the VOCs levels in highly polluted cities show how different environments at different times of the day have varying levels of different VOCs [14].

Since 2010, Lithuania has been ranked among the fastest growing economies in the European Union [15], and therefore has seen an augment in the traffic. As it is common for all major cities around the world, the increase in traffic has boosted the environmental contamination, and therefore, the levels of VOCs. Several studies show how Vilnius had problems with atmospheric contamination [16, 17]. Especially in neighbourhoods like Žvėrynas [18], where many houses still use coal as a way of heating, the levels of VOC emissions were higher than the limits established by the Lithuanian Ministry of Environment.

In our study, we aim to collect the VOC pattern from several locations in the city centre and identify different emission sources influencing the air composition in Vilnius.

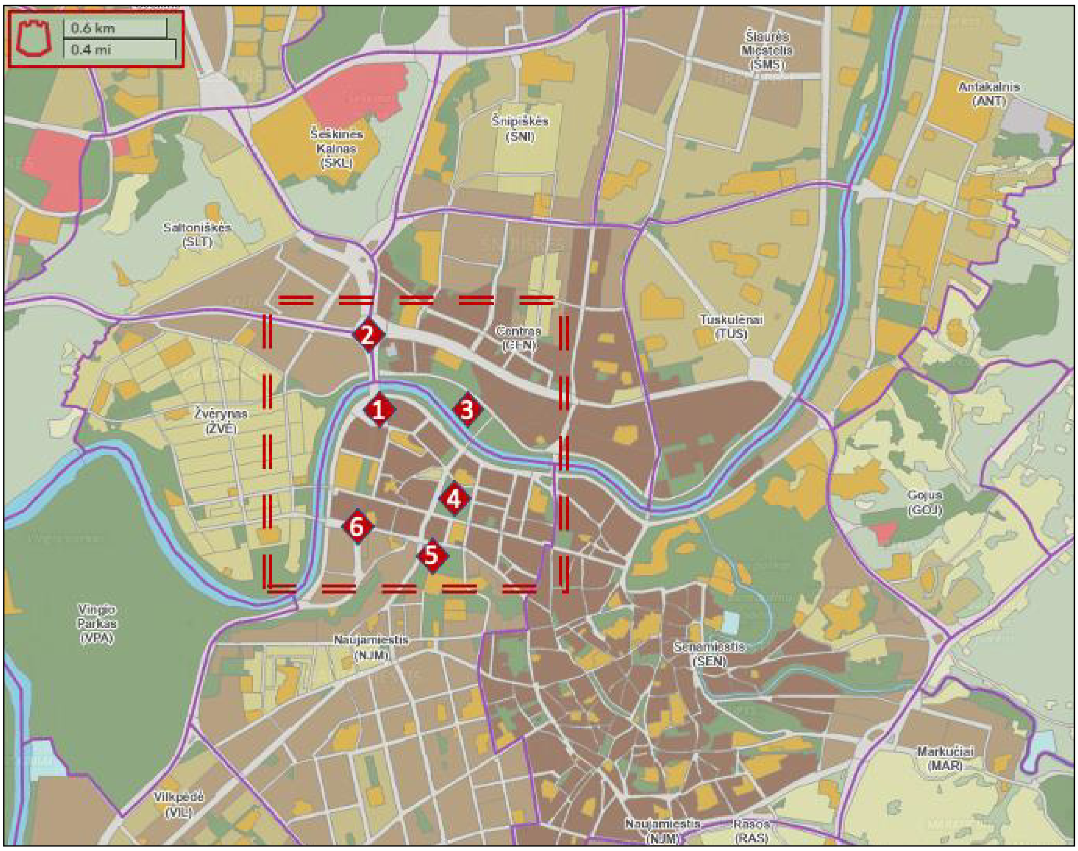
EXPERIMENTAL

Locations

We have checked the volatiles from 6 different locations in Vilnius, Lithuania. All the locations are in a 2 km^2 area within the Vilnius City center (Fig. 1). The locations were chosen with the criteria to have different traffic and greenery conditions with a variety of VOCs sources.

Equipment

Thermal desorption (TD) tubes were employed for the collection of samples. TD tubes with a Tenax® TA sorbent were purchased from Markes International (UK). The air samples were pumped through the sorbent by using an air sampler



Map legend: 1, the petrol station close to a heavy traffic road; 2, a very heavy traffic road crossing (elevated pass); 3, a large park area with a low traffic road nearby; 4, a small park area with a low traffic road nearby; 5, a small park area with a heavy traffic road nearby; 6, a very heavy traffic road (tunnel).

Fig. 1. Vilnius map with the sampling locations [from www.maps.vilnius.lt]

Aircheck Sampler model 224–44XRM from SKC Inc.

Sample collection

TD tubes were conditioned following manufacturers' instructions. Air samples were collected at the specific locations (Fig. 1) by applying a flow of 1000 ml/min for 10 min. All the samples were collected the same day, in a range of 2 h to have similar weather conditions in all the locations (Table 1). The samples were analysed within 3 h from their collection time. The samples from the same

Table 1. **Weather conditions**

Day 1 (3 August 2021)						
Time	**Temperature**	**Humidity**	**Wind**	**Wind speed**	**Precip.**	**Condition**
10:20 AM	17°C	77%	WSW	17 km/h	0.0 mm	Mostly cloudy
10:50 AM	16°C	88%	WSW	15 km/h	0.0 mm	Light rain shower
11:20 AM	18°C	83%	WSW	19 km/h	0.0 mm	Mostly cloudy
11:50 AM	18°C	73%	W	17 km/h	0.0 mm	Mostly cloudy
Day 2 (20 August 2021)						
Time	**Temperature**	**Humidity**	**Wind**	**Wind speed**	**Precip.**	**Condition**
10:20 AM	19°C	60%	WSW	17 km/h	0.0 mm	Fair
10:50 AM	20°C	56%	WSW	19 km/h	0.0 mm	Mostly cloudy
11:20 AM	20°C	60%	SW	20 km/h	0.0 mm	Mostly cloudy
11:50 AM	20°C	60%	WSW	19 km/h	0.0 mm	Mostly cloudy
Day 3 (23 August 2021)						
Time	**Temperature**	**Humidity**	**Wind**	**Wind speed**	**Precip.**	**Condition**
10:20 AM	19°C	56%	SSW	7 km/h	0.0 mm	Fair
10:50 AM	20°C	52%	VAR	7 km/h	0.0 mm	Partly cloudy
11:20 AM	18°C	56%	W	6 km/h	0.0 mm	Mostly cloudy
11:50 AM	19°C	56%	VAR	6 km/h	0.0 mm	Mostly cloudy
Day 4 (24 August 2021)						
Time	**Temperature**	**Humidity**	**Wind**	**Wind speed**	**Precip.**	**Condition**
10:20 AM	15°C	63%	NNE	17 km/h	0.0 mm	Partly cloudy
10:50 AM	15°C	63%	NNE	19 km/h	0.0 mm	Mostly cloudy
11:20 AM	15°C	59%	N	22 km/h	0.0 mm	Partly cloudy
11:50 AM	16°C	55%	NNE	20 km/h	0.0 mm	Partly cloudy
Day 5 (25 August 2021)						
Time	**Temperature**	**Humidity**	**Wind**	**Wind speed**	**Precip.**	**Condition**
2:50 PM	17°C	52%	W	17 km/h	0.0 mm	Mostly cloudy
3:20 PM	17°C	52%	SW	19 km/h	0.0 mm	Mostly cloudy
3:50 PM	16°C	55%	WSW	15 km/h	0.0 mm	Mostly cloudy
4:20 PM	17°C	52%	WSW	13 km/h	0.0 mm	Mostly cloudy
Day 6 (7 September 2021)						
Time	**Temperature**	**Humidity**	**Wind**	**Wind speed**	**Precip.**	**Condition**
10:20 AM	15°C	55%	SW	13 km/h	0.0 mm	Fair
10:50 AM	15°C	55%	SSW	15 km/h	0.0 mm	Fair
11:20 AM	16°C	48%	SW	15 km/h	0.0 mm	Fair
11:50 AM	16°C	45%	WSW	15 km/h	0.0 mm	Fair

Source: www.wunderground.com. The Weather Company, an IBM business.

exact locations were collected during 6 different days to compare the variations of the VOC profile.

Weather conditions

The weather conditions for the 6 days when the samples were collected are presented in Table 1.

Sample analysis

TD tubes were loaded into the TD system (ATD 400, Perkin Elmer) where the tubes were heated, releasing the trapped compounds into the system using the parameters from Table 2. The compounds were then separated and identified using a GC-MS system (Agilent 6890N coupled to a mass spectrometer AutoSpec Premier, Waters/Micromass). The DB-5MS, 30 m, 0.25 mm ID, 0.25 mm (Agilent Technologies) column temperature was held at 40°C for 3 min and was then increased by 5°C/min to 120°C, followed by ramping at 10°C/min to 220°C. The MS analyses were performed in the full-scan mode, using a scanning range *m/z* 50–200. The ion source was maintained at 250°C, and ionization energy (EI+) of 70 eV was used for each measurement. Compound identification was performed by the library match using the NIST MS Search 2.0 (2005) mass spectral library. Data statistical analysis was performed using the R Core Team, the jamovi project and OriginLab software [19, 20].

Table 2. **Thermal desorption system (ATD 400) parameters**

Carrier gas	Helium 5.0	**Oven temp.**	220°C
Desorption flow	60 mL/min	**Oven hold**	5 min
Outlet split	6 mL/min	**Trap temperature**	280°C
Inlet split	No	**Trap hold**	3 min

RESULTS AND DISCUSSION

The compounds from all the locations were identified and their relative concentration was obtained by collecting the areas from the chromatograms (Table 3). In an area of two square kilometers we found different sources of VOCs; each area gave a distinctive pattern of compounds (Fig. 2).

Table 3. **Main compounds identified in the locations studied and their average relative concentration for each location**

Ret. time	Compound	Possible sources	Loc. 1 Rel. %	Loc. 2 Rel. %	Loc. 3 Rel. %	Loc. 4 Rel. %	Loc. 5 Rel. %	Loc. 6 Rel. %
1.00	Acetone	Petrol/car exhaust/human breath	6.24	8.08	9.95	6.73	5.57	5.79
1.13	tert-Butyl methyl ether	Fuel additive	5.67	2.42	2.75	2.32	2.48	2.67
1.40	*Benzene	Petrol/car exhaust	4.68	5.77	3.83	4.79	4.92	5.24
1.59	Heptane	Fuel additive	1.93	2.47	2.90	3.05	3.01	3.05
1.81	Butyl octanol	Petrol/car exhaust	0.51	0.87	0.70	0.89	0.76	0.83
1.98	Hexone	Other	0.45	0.59	0.64	0.80	0.55	0.55
2.24	*Toluene	Petrol/car exhaust	20.65	18.12	12.65	15.03	17.78	17.42
2.72	Octane	Petrol/car exhaust	0.93	0.53	0.70	0.50	0.79	3.29
3.05	Butyl acetate	Fragrances	1.02	2.92	2.97	1.70	1.56	1.31
3.97	*Ethyl benzene	Petrol/car exhaust	3.83	3.94	2.94	3.07	3.73	4.07
4.22	*m, p xylene	Petrol/car exhaust	12.99	11.66	8.85	9.55	12.69	13.12
4.77	*o xylene	Petrol/car exhaust	4.57	5.22	3.58	4.30	5.01	5.41
5.84	#a-pinene	Vegetation/fragrances	2.90	4.46	6.79	5.35	3..03	3.01
6.31	#Camphene	Vegetation/fragrances	1.05	0.67	1.06	0.56	0.80	<LOD
6.41	Dimethylolpropane	Other	8.46	<LOD	<LOD	<LOD	<LOD	<LOD
6.54	*Propyl benzene	Petrol/car exhaust	1.10	1.13	1.19	0.59	0.93	0.96
6.74	*1,2,4-Trimethylbenzene	Petrol/car exhaust	2.37	1.87	2.74	1.28	2.43	2.33
6.85	*m-Ethyltoluene	Other	1.29	0.78	2.57	1.00	0.92	1.04

Table 3. **(continued)**

Ret. time	Compound	Possible sources	Loc. 1 Rel. %	Loc. 2 Rel. %	Loc. 3 Rel. %	Loc. 4 Rel. %	Loc. 5 Rel. %	Loc. 6 Rel. %
6.90	Benzaldehyde	Vegetation/fragrances	2.57	6.03	6.74	9.40	5.05	3.98
7.14	#4-Carene	Vegetation/fragrances	0.61	0.90	2.19	3.38	<LOD	<LOD
7.23	*p-Ethyltoluene	Petrol/car exhaust	0.83	0.97	2.06	0.58	0.90	1.13
7.72	*1,2,3-Trimethylbenzene	Petrol/car exhaust	3.79	3.49	2.88	3.20	3.86	3.61
8.02	4-Ethyloctane	Petrol/car exhaust	0.79	1.10	0.88	1.23	1.11	1.30
8.14	#Terpinen	Vegetation/fragrances	1.31	3.19	9.31	7.20	2.94	1.58
8.22	Octanal	Petrol/car exhaust	0.74	0.53	1.43	1.69	1.03	0.77
8.53	*1,3,5-Trimethylbenzene	Petrol/car exhaust	0.76	0.94	1.29	0.73	0.87	1.12
8.85	#D-Limonene	Vegetation/fragrances	0.55	0.68	2.27	1.50	0.89	0.47
8.90	p-Methylstyrene	Other	0.59	0.73	0.54	0.90	0.62	0.74
9.03	2-Ethyl-1-decanol	Other	0.55	0.63	1.03	1.16	0.96	1.00
9.42	*1,3-Diethylbenzene	Petrol/car exhaust	0.14	0.41	<LOD	<LOD	0.28	<LOD
9.51	*1-Methyl-3-propylbenzene	Petrol/car exhaust	0.58	0.83	<LOD	<LOD	0.64	0.80
9.68	*1-Methyl-2-propylbenzene	Petrol/car exhaust	0.43	1.07	<LOD	<LOD	0.71	1.05
9.72	*2-Ethyl-1,4-dimethylbenzene	Petrol/car exhaust	0.83	1.02	<LOD	<LOD	1.46	1.10
9.90	2-indanol	Other	0.51	0.43	0.65	<LOD	0.37	0.32
10.11	Acetophenone	Vegetation/fragrances	1.89	3.80	4.35	4.57	2.62	2.29
10.28	*1,2-Dimethyl-4-ethylbenzene	Petrol/car exhaust	0.38	1.93	<LOD	<LOD	1.08	1.52
10.36	*1-Ethyl-2,4-dimethylbenzene	Petrol/car exhaust	0.68	0.78	<LOD	1.19	0.72	0.56
10.53	*1,2,4,5-Tetramethylbenzene	Petrol/car exhaust	0.60	1.30	<LOD	0.67	0.93	0.77
11.13	Undecane	Other	1.27	1.37	1.08	1.15	1.27	1.90
11.38	Nonanal	Fragrances/human breath	5.80	2.51	4.84	3.28	4.73	3.08
11.52	*1,2,3,4-Tetramethylbenzene	Petrol/car exhaust	0.17	0.66	<LOD	<LOD	0.22	0.58
11.59	*1,2,3,5-Tetramethylbenzene	Petrol/car exhaust	0.48	0.66	<LOD	<LOD	0.65	0.70
12.42	4-Methylindane	Other	0.52	0.38	<LOD	<LOD	<LOD	<LOD
12.51	*1,2-Dimethyl-3-ethylbenzene	Petrol/car exhaust	0.29	0.76	<LOD	<LOD	0.31	0.47
13.53	1-Methylene-1H-indene	Other	0.65	1.41	1.23	1.13	0.96	1.53
14.18	6-Methyltridecane	Other	1.01	2.00	1.21	1.79	1.16	1.80
14.44	Decanal	Vegetation/fragrances	0.98	1.88	2.71	3.34	2.98	1.42
14.89	Benzothiazole	Fragrances	0.56	1.45	0.83	1.19	1.26	1.40
15.03	Cyclohexyl isothiocyanate	Other	0.66	1.19	1.39	1.41	1.90	1.12
16.58	#Isobornyl acetate	Vegetation	0.97	0.81	3.75	1.33	0.30	0.42
17.06	Tridecane	Petrol/car exhaust	1.05	1.25	1.19	1.25	1.16	1.50
	* Total benzene derivates		58.88	55.97	37.05	41.93	54.76	57.41
	#Total terpenes		4.71	8.10	22.11	14.43	6.75	4.97

<LOD: below the limit of detection.

As we collected the volatiles from those locations during several days, we could identify the punctual events happening in each location: re-fuelling the petrol station (Fig. 3), cutting the grass and installation of new benches (newly painted). Meteorological events also affected the results; during a windy day, the composition of VOCs was diluted, obtaining a decrease in the levels of compounds (Fig. 4).

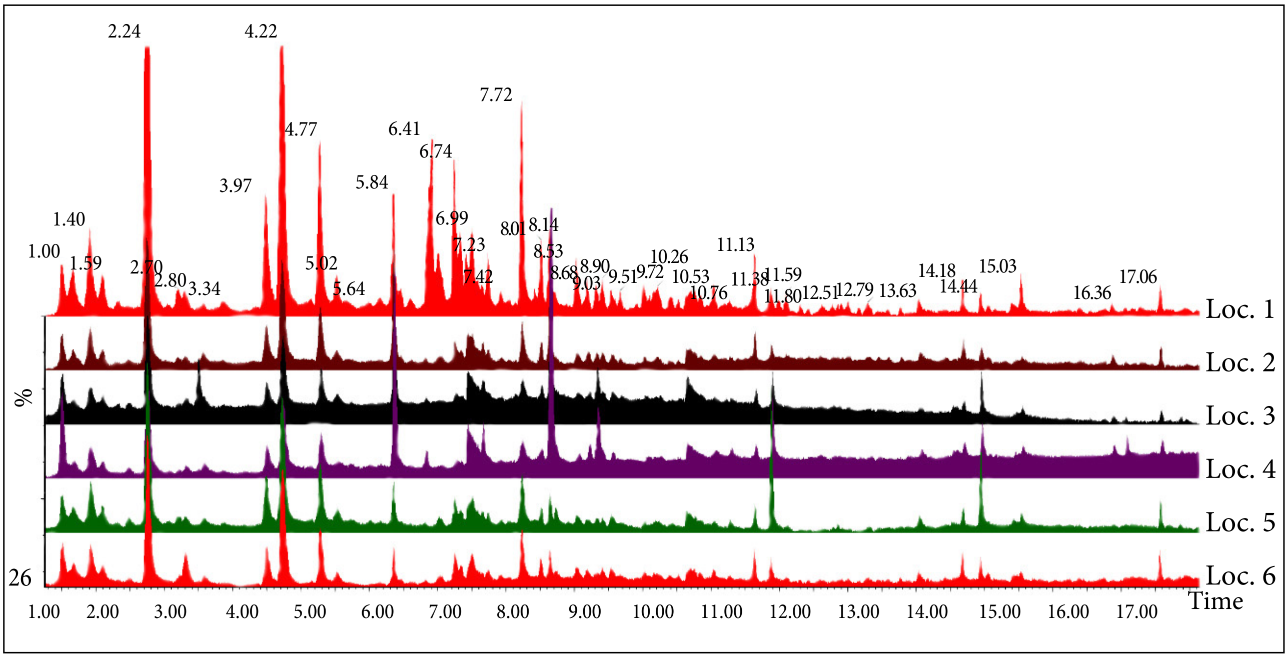


Fig. 2. Chromatogram from the 6 locations (same day)

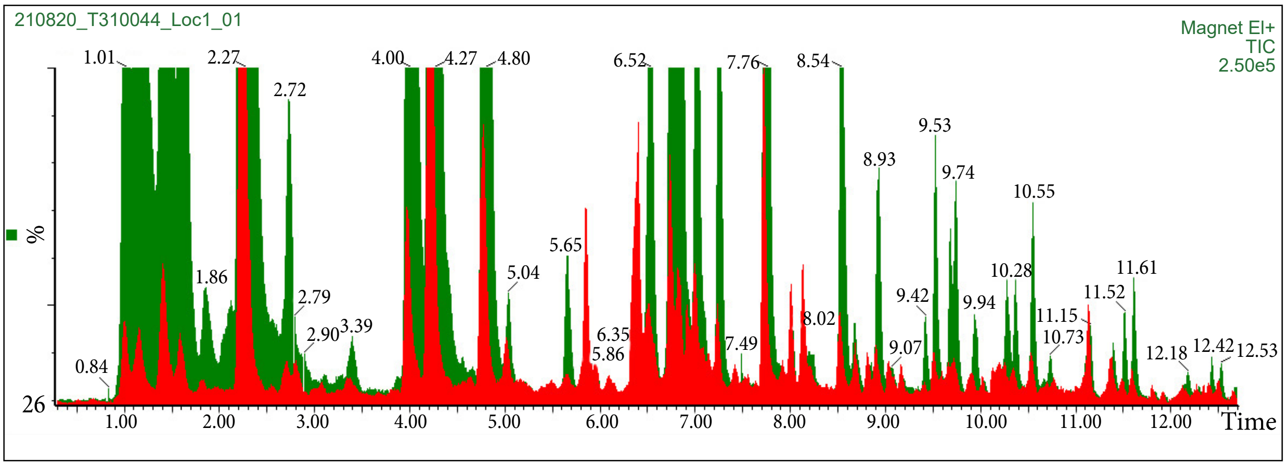


Fig. 3. Increase of VOC levels when re-fuelling petrol. Green: re-fuelling event, Location 1 (Day 2); red: usual day, Location 1 (Day 6)

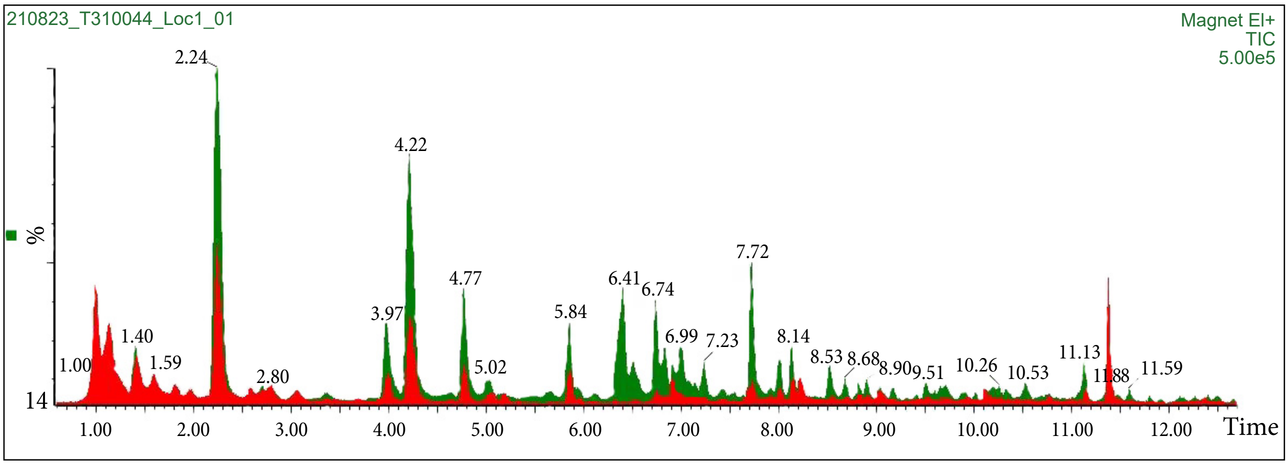


Fig. 4. Decrease of VOC levels on a windy day. Green: wind speed 7 km/h, Location 1 (Day 3); red: wind speed 17 km/h, Location 1 (Day 1)

Even though the levels of VOCs might differ depending on various factors and weather conditions, we studied the full profile for each location. We calculated the average relative concentration of VOCs for the 6 different locations during all the sampling days (Table 3).

Principal component analysis (PCA) was performed to decrease the amount of variables (Fig. 5). The data showed that the main difference across the locations was the presence of benzene derivates and terpene compounds. The park locations have a higher concentration of biogenic VOCs (terpenes), while the locations with intense traffic have a higher concentration of anthropogenic VOCs (benzene derivates). Therefore, we decided to group those variables to perform ANOVA analysis (Fig. 6).

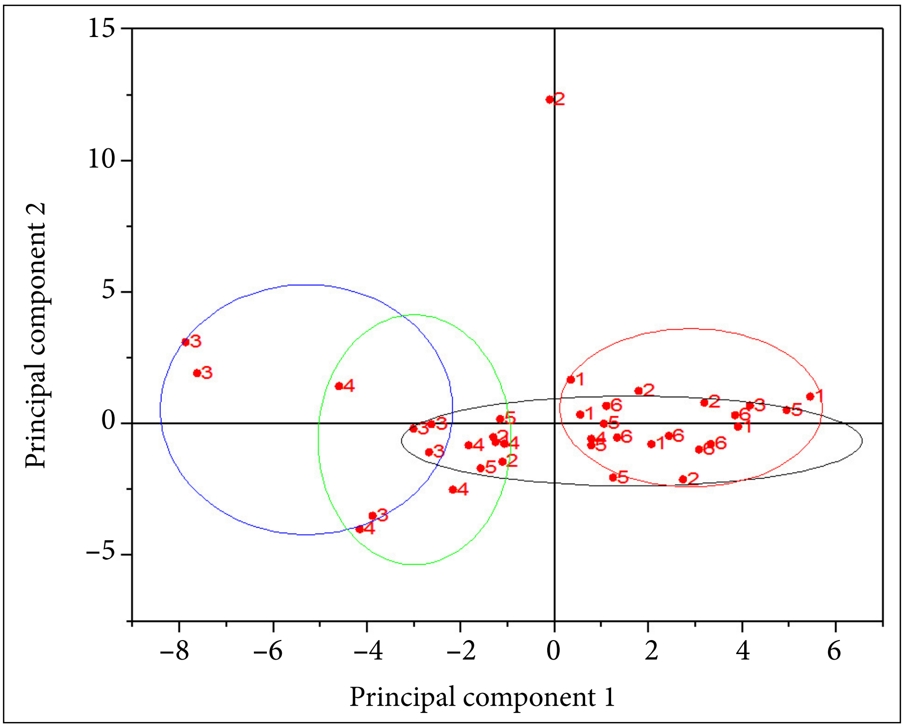


Fig. 5. PCA analysis. Clusters: red: Locations 1, 2 and 6; blue: Location 3; green: Location 4; black: Location 5

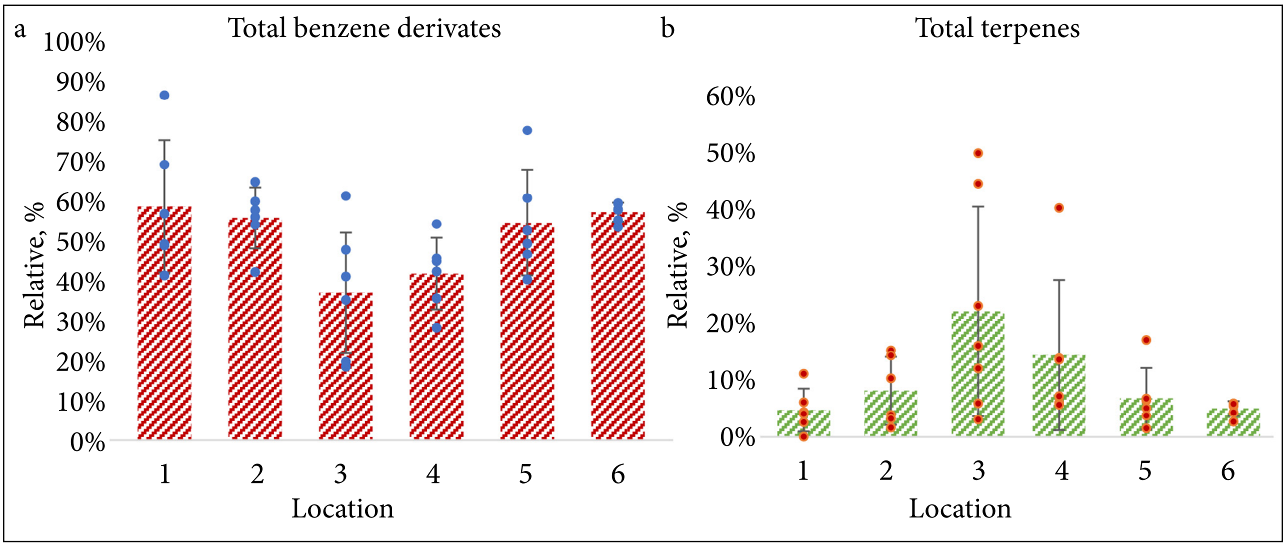


Fig. 6. Relative concentration of total benzene derivates (a) and total terpenes (b) for each location. Column graph: total average; scatter graph: daily value

However, a big variance of the results might be a problem to get statistically significant differences. We firstly performed the Levene's test (Table 4) for the analysis of variance homogeneity and the Shapiro–Wilk test (Table 5) for the study of the normal distribution of the results. Looking at the test results we cannot assume a normal distribution of the results for the total terpene concentration nor assume equal variances. Because of that, we performed Welch's One-way ANOVA for total terpenes, and Fisher' One-way ANOVA for total benzene derivates (Table 6).

Table 4. **Homogeneity of Variances Test (Levene's)**

	F	df1	df2	*p*
Terpenes	4.72	5	31	0.003
Benzene derivates	2.18	5	31	0.082

Table 5. **Normality Test (Shapiro–Wilk)**

	W	*p*
Terpenes	0.868	<.001
Benzene derivates	0.949	0.087

Note. A low *p*-value suggests a violation of the assumption of normality.

Table 6. **One-way ANOVA**

		F	df1	df2	*p*
Terpenes	Welch's	1.81	5	13.0	0.180
Benzene derivates	Fisher's	3.82	5	31	0.008

The analysis shows a non-statistically significant result for total terpene concentration for the 6 locations (p = 0.180), but a statistically significant result for total benzene derivates concentration (p = 0.008).We finally performed a Tukey (equal variances) Post-Hoc Test (Table 7) to identify in which locations the results were statistically significantly different. Only the locations 4 and 6 show a statistically different result.

CONCLUSIONS

We analysed the VOC content and their relative concentrations in 6 different locations in Vilnius within an area of 2 km^2. The results show a tendency which areas with a higher traffic load (Locations 1, 2 and 6) have a higher concentration of anthropogenic VOCs. In addition to that, the levels of biogenic VOCs were higher in the locations dominated by greenery (Locations 3 and 4). Location 5 (a park with heavy traffic) has a mix of both conditions, therefore the weight of anthropogenic and biogenic VOCs is similar. We observe a very disperse variation of the results for each location. This is due to a number of parameters that could affect the results: punctual events like re-fuelling in a petrol station, cutting the grass, fumigating plants, traffic conditions, installation or renewal of urban furniture, as well as weather conditions like air temperature, wind speed, wind direction or rain. Due to these variations and data that contain a large number of outliers, we could not establish

Table 7. **Games–Howell Post-Hoc Test – benzene derivates**

			1	**2**	**3**	**4**	**5**	**6**
1	Mean difference	–	2.91	21.8	16.95	4.12	1.47	
	p-value	–	0.998	0.224	0.338	0.996	1.000	
2	Mean difference		–	18.9	14.04	1.21	−1.44	
	p-value		–	0.127	0.120	1.000	0.997	
3	Mean difference			–	−4.89	−17.72	−20.36	
	p-value			–	0.976	0.293	0.080	
4	Mean difference				–	−12.83	−15.48	*
	p-value				–	0.431	**0.050**	
5	Mean difference					–	−2.65	
	p-value					–	0.995	
6	Mean difference						–	
	p-value						–	

Note. * $p < .05$.

statistically significant results. We could not establish that the differences in VOCs compositions across locations were statistically significant. However, we still observed differences in VOCs compositions across the six locations. This shows that even though the area of sampling was rather small, the different sources of VOCs have a strong influence in the air composition. This difference in the air composition allows us to discriminate different environments in the city.

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LAKIŲJŲ ORGANINIŲ JUNGINIŲ PROFILIAVIMAS SKIRTINGAI APLINKAI IDENTIFIKUOTI VILNIAUS MIESTE

Santrauka

Šio tyrimo tikslas buvo parodyti, kad lakiųjų organinių junginių (LOJ) profiliavimas gali būti naudojamas kaip būdas identifikuoti skirtingas miesto aplinkas. Norėdami tai pasiekti, taikėme kelis metodus. Pirmiausia atlikome LOJ profilio matavimus keliose skirtingose vietose. Tada nustatėme potencialių žymenų junginius ir jų šaltinius. Oro ėminiai buvo paimti iš šešių skirtingų Vilniaus miesto vietų, naudojant terminės desorbcijos (TD) vamzdelius. Ėminiai buvo išanalizuoti dujų chromatografijos-masių spektrometrijos metodu, naudojant termodesorbcinį mėginių įvedimą (TD/DCh-MS). Junginiai buvo identifikuoti pasitelkiant *NIST MS Search 2.0* (2005) masių spektrų biblioteką. Rezultatai parodė skirtingus LOJ lygių rezultatus santykinai mažame 2 km^2 plote, priklausomai nuo skirtingų emisijos šaltinių, kuriuos galima naudoti skirtingai aplinkai identifikuoti.