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CHARACTERIZATION OF VOLATILE ORGANIC COMPOUNDS OF ESSENTIAL OILS PRODUCED IN TRIESTE KARST AREA BY HS-SPME-GC-MS AND COMPARISON WITH AN ELECTRONIC NOSE DISCRIMINATION POTENTIAL FOR QUALITY CONTROL PURPOSES

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According to the Commission of the European Pharmacopoeia [1] an essential oil is an "*odorous product, usually with a complex composition, obtained from a botanically defined plant raw material by steam distillation, dry distillation, or a suitable mechanical process without heating Essential oils are usually separated from the aqueous phase by a physical process that does not significantly affect their composition*".
Essential oils can be constituted by a variety of volatile organic compounds such as terpenes, alcohols, aldehydes, ketones, phenols, esters, ethers, oxides, peroxides, furans, organic acids, lactones, and sulfur compounds. Factors such as climate, soil, genetic features, and cultivation techniques greatly influence their composition in different plant species [2].
Since there is a growing interest in the use of essential oils as e.g. antimicrobial, insecticide, antiseptic, antifungal, and analgesic activities, aromatherapy, and disease treatments, there is the need of quality control for safety use starting from the raw material throughout the production process. Moreover essential oils can also be produced from different chemotypes which provide distinct chemical entities within the same botanical species [3].
Different chemotypes of the same species can show different activities in relation with the purpose and, in some cases a specific chemotype can contain toxic substances thus the use have to be avoided. The differences in chemotypes can be associated e.g. to the geographical area, the plant harvesting period and the vegetation environment [4]. Therefore there is the need of an extended characterization for quality control.
The aim of this study is the qualitative chemical characterization of essential oils produced in Trieste Karst area. Essential oils produced starting from thirteen plant species has been characterized by HS-SPME-GC-MS.
Nearly 280 compounds have been identified by a mixed use of: matching with mass spectra databases, Linear Retention Index and standard compounds.

O2 EAC3

N	t.r. (min)	Compound	CAS	L.R.I.	Identification
1	5,7776	3-Pentanone 2,2-dimethyl-	564-04-5	839	LRI
2	5,9647	Butanoic acid 2-methyl-ethyl ester	7452-79-1	847	LRI
3	6,035	Cyclohexane ethylidene	1003-64-1	850	MS
4	6,0583	3-Octen-2-ol (E)	57648-55-2	851	MS
5	6,0816	Butanoic acid 3-methyl-ethyl ester	108-64-5	852	LRI
6	6,1285	Cyclopentane 1,1-dimethyl-	1638-26-2	854	MS
7	6,2454	2,4-Nonadiene (E)-	56700-78-8	859	MS
8	6,2454	Ethanone 1-(2-methyl-1-cyclopenten-1-yl)-	3168-90-9	859	MS
9	6,4561	1-Hexanol	111-27-3	868	LRI
10	6,713	1-Butanol 2-methyl- acetate	624-41-9	878	LRI

Figure 1. Part of the compound identification table (overall = 280 compounds)

73 compounds were found to be useful in identifying differences between species. Moreover we identified possible compounds related to the "Karst" chemotype comparing the results with those present in scientific literature.

N	t.r. (min)	Compound	CAS	C1	C2	C3	C4	C5	C6	C7	C8	C9
1	5,7776	3-Pentanone 2,2-dimethyl-	564-04-5						x			
2	5,9647	Butanoic acid 2-methyl-ethyl ester	7452-79-1		x							
3	6,035	Cyclohexane ethylidene-	1003-64-1				x					
4	6,0583	3-Octen-2-ol (E)	57648-55-2			x						
5	6,0816	Butanoic acid 3-methyl-ethyl ester	108-64-5		x					x		
6	6,1285	Cyclopentane 1,1-dimethyl-	1638-26-2				x					
7	6,2454	2,4-Nonadiene (E)-	56700-78-8			x						
8	6,2454	Ethanone 1-(2-methyl-1-cyclopenten-1-yl)-	3168-90-9				x					
9	6,4561	1-Hexanol	111-27-3	x			x					
10	6,713	1-Butanol 2-methyl- acetate	624-41-9						x			

Figure 2. Part of the presence/absence table for essential oil comparison (overall = 73 compounds)

The essential oil VOC profiles have been also analyzed by a 32 sensors array electronic nose to correlate the sensor signals to the chemical characterization and evaluate the e-nose discrimination potential. The data have been elaborated by Principal Component Analysis.

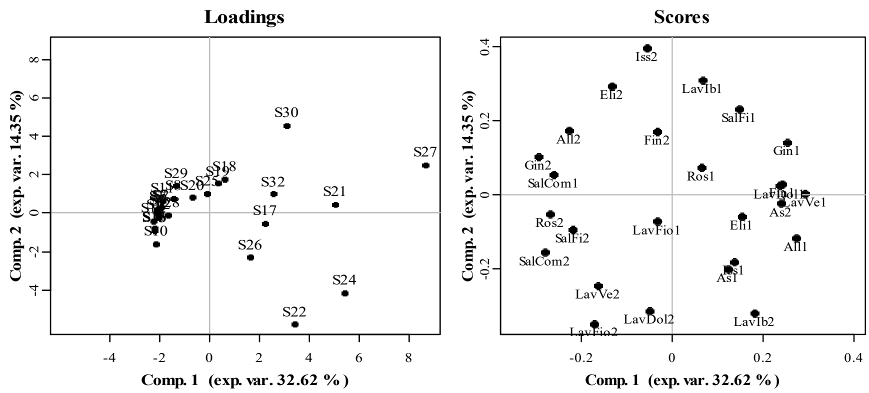

Figure 3. Principal Component Analysis of the electronic nose data.

References
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