

SUMMARY
PhD THESIS

STUDY OF VOLATILE CONGENERS IN ALCOHOLIC BEVERAGES

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INTRODUCTION

By definition, any liquid that is drinkable and its content of ethyl alcohol ranges from 0.5% to 95 % is an alcoholic beverage. Although ethyl alcohol is the major component of most alcoholic beverages, there is a remaining fraction of compounds called generic congeners. Even if the amount of these quantities are small, they play an important role in social issues related to the use or misuse of alcohol.

While thousands of different volatile congeners may be found in various alcoholic drinks, at a time it was noted that there are some which are constantly present: methyl alcohol, acetone n-propanol, isobutanol, n-buthanol, 2-butanol, 2-methyl-1-butanol; some volatile congeners have important role in the composition of certain drinks such as beer, wine and distilled spirits.

Keywords: beverages, volatile congeners, validation

PERSONAL CONTRIBUTION

All laboratory tests comprising a total amount of 1,250 analysis were performed using the "Konica HRGC 4000B" gas chromatography device- manufactured in Spain and equipped with a FID (flame ionization) detector and a "Carbowax" - 2.0 μ m - 30m - 0.53 mmID capillary column.

1 Development and validation of a gas chromatographic method used in order to determine the volatile congeners in alcoholic beverages. The retention times for the following congeners in alcoholic beverages were identified: acetone, methanol, 2-butanol, n-propanol, isobutanol, 1-butanol, 2-methyl-1-butanol, using the gas chromatographic method. The following validation parameters were determined: linearity, limit of detection, limit of quantification, precision accuracy.

2 Analysis of alcoholic beverages. A number of alcoholic beverages were analyzed and were classified into: distilled beverages, wine, beer and some imported drinks used for a comparative study. Distilled alcoholic beverages based on fermented fruits are rich in congeners while distillates obtained from the fermentation of grain are much cleaner (vodka, gin). Distilled spirits produced in households (țuica = brandy), generally have a higher content of methanol compared to distillates (vinars=brandy) obtained using more elaborate procedures.

Tabel III.3.3 Volatile congeners in Romanian beverages (mg/L)

Beverages	Aceton mg/L	Methanol mg/L	2- butanol mg/L	n- propanol mg/L	Isobuthanol mg/L	1- butanol mg/L	2-metil- 1- butanol mg/L
Vinars(brandies)	0.5 – 12.36	24.09- 892.91	6.96- 11.65	74.13- 219.16	0.74-318.35	0.73- 44.54	9.96- 1055.2
Home made spirits	1.04- 22.45	34.79- 2877.97	105.96- 129-45	166.35- 520.10	81.16- 259.56	20.27- 101.92	34.05- 601.61
Beer	0 – 4.7	0.98-43.8	-	1.62- 70.91	1.59-21.82	0 -3.8	1.97- 52.41
White wine	1.05- 15.55	59.15- 132.44	-	6.42- 57.86	0.46-66.52	9.68- 33.36	101.67- 178.51
Red wine	3.08- 11.62	122.05- 366.78	-	10.61- 58.9	16.63-43.37	0 -16.47	171.57- 324.09

3. The analysis of the principal component (APC) was applied to two categories of distilled beverages produced in Romania, namely “vinarsuri” (brandies) and home-made spirits from Transylvania. This is a very useful statistical method to define a model (pattern) in our case for various alcoholic drinks. APC is a tool designed to identify unknown trends in a set of multidimensional data. The implementation of the analysis of the principal component is equivalent to applying the mathematical model of singular value decomposition (SVD). The application of singular value decomposition shows that between the converted coordinates (principal components – PC -) there are finally linear combinations. Methanol and amyl- alcohol are the main components that determine the difference between these beverages. Any change in the content of one component leads to changes in the other one. Alcoholic beverages obtained by controlled methods in terms of manufacturing conditions have a constant behavior as respects the analysis of the principal component than the beverages obtained in households.

4 The determination of volatile congeners from biological samples. The aim was to develop a qualitative and quantitative identification method of volatile congeners in blood taken from drivers caught in traffic under the influence of alcohol, and biological samples taken during autopsies of suspicious deaths (blood, urine, gastric contents, etc.)

The validation parameters were: linearity, the limit of detection, the limit of quantification, accuracy, precision. The accuracy was within the of range ± 0.009 (methanol) - ± 0.184 (2-butanol).The accuracy of relative standard deviation (RSD) is in the range of 5.30% (1-butanol) -8.41 (n-propanol)

Measurements of volatile compounds in blood taken from apprehended drivers in traffic is important in the development of certain expertise concerning a more complex alcohol consumption and which should confirm or not the statements with reference to alcohol consumption. Isobutanol and n-propanol compete in terms of elimination. 2-butanol appears particularly in distillates obtained from fruits - the emergence during the analysis is almost certainly an indication of the consumed alcoholic beverages, but its presence in the blood taken after autopsy should be taken into consideration because some authors consider 2-butanol as a marker of rotting.

The characterization of alcoholic beverages regarding their content of volatile congeners, and the composition of tables containing volatile congeners are particularly useful in order to know the quality of alcoholic beverages and thus to ensure that these compounds are in normal limits according to the requirements of the European Communities. Working with a validated method of analysis, the tables can be filled continuously. It is also possible to develop cooperation programs with the Department of Consumer Protection in order to detect counterfeit alcoholic beverages to those declared by the manufacturer.

Being aware of the content of congeners in alcoholic beverages can be a starting point to conduct more complex forensic expertise with respect to alcohol consumption in individuals caught in traffic under the influence of alcoholic beverages.