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An analytical hierarchy process for selection of the optimal procedure for resveratrol determination in wine samples

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ABSTRACT

The study shows the application of analytical hierarchy process (AHP) in ranking the analytical procedures, that are applied for resveratrol determination in wine samples. 19 different analytical methodologies are described by metrological, economic and environmental criteria, that are further divided into 10 subcriteria. Before AHP application, the amount of input data is decreased with cluster analysis. The first run of AHP is aimed to rank the clustered analytical procedures, while the second analysis is performed to select the best procedure from the cluster with the highest rank obtained in the first AHP run. The procedure based on a direct sample injection to high performance liquid chromatography with UV detection is the most beneficial one. AHP is excellent tool for the assessment and the selection of the most appropriate analytical procedure from several available. The choice of MCDA method is dictated by the fact, that so far, no examples of the usage of a given method for the selection of the optimal analytical procedure have been found in the literature.

1. Introduction

Without a doubt, the relationship between diet and health has developed an intense research in bioactive compounds in foods. Among food and beverages products, wine seems to be an essential component and may be partially responsible for health-promoting properties. Wine, especially the red variety, has been studied extensively over many years. It is well known, that moderate consumption of red wine, is associated with several potential health benefits, such as lower risk of cardiovascular or neurological diseases and anti-cancer properties [1].

The most significant and beneficial health properties of wine consumption are related to compounds with high antioxidant capacity like polyphenols, including trans-resveratrol [1].

Resveratrol is a phenolic compound, occurring naturally in overground part of plants, mainly in seeds, skin and leaves. It is synthesized from phenylalanine through the shikimic pathway and three key enzymes are involved in this pathway: coenzyme A ligase, phenylalanine ammonium lyase, and stilbene synthase. The biosynthesis of these enzymes can be induced by stress, thus resveratrol is a phytoalexin synthesized by grapes after exposure to biotic or abiotic stress [1]. Therefore, it can be stated, that resveratrol is produced in grapes as self-protection against toxins and it can be found within the skins [2]. The persistence of the grape skins during the fermentation process impacts on the resveratrol content in final products, meaning wines. The concentration of this compound is lower in white wine than in red wine, due to the fact, that skins are removed earlier during production of the white wines [3].

Resveratrol has recently been the subject of intensive investigation. This is mainly due to being reported as a potent antioxidant, anticancer, anti-inflammatory and chemoprotective agent. Moreover, this compound is associated with increased longevity, and cardiovascular protective effects, due to its ability to reduce platelet aggregation, modulate lipid metabolism, and inhibit oxidation of low density lipoprotein [4,5]. The increased awareness of the trans-resveratrol beneficial impact on human health and the challenges associated with its low and variable abundance in samples characterized by complex matrix composition, have driven the need to develop rapid and reliable methods for resveratrol analysis in wine and related samples. Many analytical procedures have been developed for determination of resveratrol in wine, which are based on the application of gas chromatography (GC), high performance liquid chromatography (HPLC) and capillary electrophoresis (CE) [6–9]. Pre-concentration step is often required, because resveratrol occurs at low concentration level as well as, because wine is characterized by complex matrix composition. However, several direct methods are also reported. Taking into consideration separation and determination technique, derivatization process is often required to:

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- increase volatility and thermal stability of analytes, improve resolution as well as detection parameters when the gas chromatography is applied;
- improve sensitivity and separation properties when the liquid chromatography is utilized;
- give charge to a specific components, while using electrophoresis [10].

Some articles report application of combination of analyte preconcentration, extraction and derivatization, what is in accordance with green analytical chemistry, which arise from the principles of sustainable development [3].

Although, there is a large number of reports in the literature, which show the results of the determination of resveratrol compound in the wine industry, there is a lack of critical comparisons of developed methodologies, not only in terms of the parameters of the analytical merits achieved, but also in terms of their green character. It is clear, that analytical procedure for resveratrol determination should meet green analytical chemistry requirements. The large number of available procedures requires the application of dedicated tools for systematic procedure selection within complex criteria and many alternatives [3].

The approach, that gives the possibility to assess the analytical procedures taking into account their environmental impact is Multicriteria Decision Analysis (MCDA). The group of MCDA tools may be applied to select the most preferred procedure and/or rank the remaining ones [11,12]. MCDA is used to select the most appropriate procedure to determine aldrin in water samples, with green analytical chemistry principles taken into consideration in another study [11]. The ranking of analytical procedures is obtained with Preference Ranking Organization METHod for Enrichment of Evaluations (PROMETHEE). In different study, with this MCDA technique completely different weighting criteria are applied to investigate the influence of metrological, economic and environmental factors on the final ranking results [12]. Another MCDA tool - Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) is used for the assessment of analytical procedures, that are applied for the determination of ibuprofen in wastewater samples [13]. It should be emphasized that MCDA and chemometrics/multivariate statistics have different jargons. The equivalents of variables and objects known in chemometrics, in MCDA are criteria and alternatives.

This study aims to present the selection of analytical procedure for resveratrol determination in wine samples, from 19 available procedures, according to different decision making criteria. *Analytical Hierarchy Process (AHP)* as MCDA algorithm is applied for data analysis and its applicability is discussed. The choice of method is dictated by the fact, that so far, no examples of the usage of given method for the selection of the optimal analytical procedure have been found in the literature.

2. Materials and methods

2.1. AHP technique

The AHP is a multicriteria decision analysis techniquethat was developed by Saaty [14]. It is mainly used to aid solving complex decision making problems. In this methodology, the problem is structured in a hierarchy of different levels constituting of the main goal, criteria, subcriteria and alternatives. This structure organizes the components of the problem from the most general, placed in the upper part of the hierarchy, to the more detailed, located in the lower part. Elements from different levels are compared in pairs. It allows assessing relative preference with respect to each of the elements at the next and higher level. The intensity of preference between two elements is established on the basis of Saaty's Fundamental Scale [15]. A linear and bipolar scale consists of nine possible numeric values. Description of each degrees of a scale is presented in Table 1.

According to the given data, the degree of advantage of one element over another is determined. Value 1 means, that element A is of the same importance as B. On the other hand, 9 means total advantage A over B or vice versa. Odd steps are usually used. However, if it is not possible to make such an assessment by the decision maker, then even degrees (intermediate values) as 2, 4, 6, 8 are used. The determination of the advantage of one of the elements is based on the so-called axiom of reciprocity, that is a reverse system. If the responder considers, that object A has a very strong advantage over object B (A = 7B), then B will be 7 times weaker than A (1/7A = B).

As it was mentioned previously, AHP considers a set of evaluation criteria, and a set of alternative options among, which the best resolution is chosen. The best option is not that one, that optimizes each single criterion, but rather that one, which achieves the most suitable trade-off among the different criteria. It is important to note, that AHP allows making a good decision, even if some of the criteria are contrasting. Generally obtaining each scale's value is possible due to results from a questionnaire, that is designed to obtain Saaty's Scale values.

In this step experts experience and knowledge may be required to be used, as well as stakeholders' opinions.

More detailed description of AHP theory is available in references [18, 19]. The procedure is also described by Lin and Yang [20]. According to them, AHP algorithm can be briefly described in several simple steps as follows [18–20]:

1. Defining the problem, determining the goal of analysis and building the hierarchical structure model
First of all, the main aim of the analysis should be defined. Criteria or sub-criteria as well as alternatives should be also determined. Later, all the information should be put in hierarchy structural skeleton of AHP model. The number of hierarchies (levels) depends on the complexity of the problem that is analyzed. However, they are structured from the top with a goal, by criteria and sub-criteria on intermediate levels, till the alternatives, which are putted on the lowest level of hierarchy. In other words, they are presenting a range of information from general to more detailed one. Hierarchy system allows determining the influence possessed by the function among elements, as well as their impact on the entire system. It is the first step, and the most important at the same time. The quality of performance affects the correctness of results, especially the consistency between pair-wise comparisons of elements.
2. Establishing a pair-wise comparison matrix of the criteria
In this step, the elements of a particular level are compared pairwise, with respect to a specific element in the upper level. The purpose of such analysis is to derive the degree of relative importance among elements. In this way, it can be judged, which element is preferred and how much more it is preferred over another. First, criteria are compared pair-wise with respect to the goal, then sub-criteria (if they are defined) are compared pair-wise with respect to the criteria, and finally alternatives are compared with respect to the each sub-criteria or criteria. The priorities of the corresponding elements are possible to compute, thanks to an assessment, which uses 9-point scale proposed by Saaty [16]. It allows transforming the verbal judgments into numerical quantities representing the values. Given results may be presented in the form of judgmental matrix. It is worth to notice, that it is mostly applicable when each hierarchy does not contain more than seven elements. Otherwise, these elements should be clustered and divided into an additional hierarchy (for example by inclusion of sub-criteria). Comparison of two elements may be mathematically presented as:

$$A_{i,j} = \frac{W_i}{W_j} i, j = 1, 2, 3, \ldots, n \quad (1)$$

where $A_{i,j}$ denotes the weight exchange value of the pair-wise comparison of element e_i and e_j, and W_i and W_j denote the relative weights among elements.