

ULTRAVIOLET-VISIBLE (UV-VIS) SPECTROSCOPY AND CLUSTER ANALYSIS AS A RAPID TOOL FOR CLASSIFICATION OF MEDICINAL PLANTS

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ABSTRACT. The ultraviolet-visible (UV-Vis) spectroscopy coupled with cluster analysis (CA) was evaluated for the classification of some medicinal plants of different geographical growing area. To have a deeper view, the experiment was carried out on herbs belonging to different families. The UV-Vis spectra of hydroalcoholic extracts were acquired in the range of 200-800 nm. The hierarchical clustering analysis (HCA) was applied to the data matrix provided by unprocessed, normalized and standardized spectra respectively. Different types of distance measuring of (dis)similarity between the samples as well as different kinds of linkage or amalgamation rule were taken into account. The best results for the classification of the selected medicinal plants were obtained using *Ward's method* as the amalgamation rule combined with *1-Pearson r* clustering distance measurement. The obtained results reveal the ability of HCA with *Ward* and *1-Pearson r* algorithm to identify plant species even when the raw material has different provenience areas and different pedoclimatic growing conditions. In addition, this methodology revealed a direct link between herbs from different families.

Keywords: medicinal plants, classification/identification, UV-Vis spectroscopy, cluster analysis

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INTRODUCTION

The World Health Organization (WHO) encourages and promotes the integration of traditional medical practices into healthcare systems, and increasingly supports the countries producing medicinal plants [1]. Traditional medicine is often termed complementary or alternative medicine (CAM) and according to the WHO estimation, about 80% of the emerging world's population relies on herbal remedies (drugs) for therapy [2, 3].

Usually, the term *herbal drugs* denote medicinal plants or plant parts converted into phytopharmaceutical products (teas, tablets, tinctures and extracts) by means of simple processes involving harvesting, drying, storage, mincing/grinding, compressing or extraction of active compounds with different solvents. The parts of medicinal plants that may be used are root, leaf, flowers, fruit, seeds or even the whole plant. Regarding the composition, phytopharmaceuticals are mixtures of many compounds with the specific physiological effect that may act individually, additively, or in synergy to improve health and cure different ailments. The phyto-compounds that are responsible for the biological characteristics of plant species are the secondary metabolites. It is well known that for the same species, differences in geographical location and growing conditions may alter the composition by increasing/decreasing the content of the constituents responsible for the phytotherapeutic effect or appearance of other compounds. Also, different parts of the same plant contain different amounts of secondary metabolites. In this context, methods for correct identification/authentication and classification of plants with specific therapeutic actions are acquiring higher importance for consumers, producers, and the pharmaceutical industry. Usually, both identification and classification processes depend on the identification of physical, chemical and biochemical differences and similarities between samples [4].

Numerous analytical techniques have been developed for quality control and evaluate compliance with the standard requirements. Instead of this, the methods for classification and identification/authentication were less approached, because of the need for advanced methods for comparison of the analytical results with a huge volume of information from a database. Exploratory data analysis, unsupervised and supervised techniques are often used as pattern recognition methods for the classification of herbal products and reveal the similarities and dissimilarities of sample properties. The aim of the unsupervised pattern recognition methods is to detect similarities whereas supervised techniques make use of calibration or training sets with a priori known the information to build a classification model. Cluster analysis (CA) and principal component analysis (PCA) are widely applied for authenticating or classifying plants based on spectral data [5, 6]. The PCA method allows visualization of the difference between samples, whereas CA can classify