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BOOK OF ABSTRACTS

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region, but without any notice on safe usage. The objectives of this study were to evaluate water quality of wellspring based on physicochemical parameters: pH, TDS (total dissolved solid), TSS (total suspended solids), specific conductivity, total water hardness (ppm CaCO₃) determined by classical complexometric titrations and compared with ICP-OES analysis, as well as ICP/MS for trace analysis of micro elements.

The results of volumetric analysis of total water hardness (27.5 ppm CaCO₃) with the ratio Ca²⁺/Mg²⁺=2.57, classified investigated water sample in the type of very soft (<75 ppm CaCO₃) and were in accordance with ICP-OES analysis: 28.0 ppm CaCO₃ with slightly higher ratio Ca²⁺/Mg²⁺=3.06. The satisfactory accuracy of volumetric analysis was confirmed by Ca²⁺ content of 9.74 ppm in commercial drinking water "Rosa" (labeled 9.6 ppm Ca). For filtered sample the obtained TDS revealed 77 ppm (180 °C) correlated with results for unfiltered sample (TDS 126 ppm and TSS 47.8 ppm at 105 °C). The pH value and specific conductivity were 6.91 and 81.5 µS/cm (18.3 °C), respectively. The calculated TDS from specific conductivity was 61.2 ppm. The ion chromatography (IC) analysis for anions provided adjacent chloride and nitrate content 0.87 and 0.82 ppm, respectively and 12.57 ppm of sulphate. The results of micro elements analysis obtained by ICP/MS provided concentrations (As; Cd; Pb) lower than maximum allowable limits, confirming safe water usage of investigated adapted wellspring.

Keywords: adapted wellspring, water quality, total water hardness, TDS and TSS, anions' analysis

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Tools for Identification of Unknown Compounds After Gas Chromatographic-mass Spectrometric (GC-MS) Analysis of Urinary Volatile Organic Metabolites (VOMs)

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Volatile organic metabolites (VOMs) in human urine can be used in non-targeted metabolomics research to identify specific metabolites that may be useful as new diagnostic, predictive, and prognostic disease biomarkers. Determination of urinary metabolite profile provides novel information on phenotypic

characteristics of an organism that cannot be obtained from target measurement. The headspace-solid phase microextraction (HS-SPME) technique coupled with gas chromatography-mass spectrometry (GC-MS) proved to be the most successful in VOMs analysis. After data processing of raw GC-MS data crucial step is to identify compounds of interest. Due to the complexity of the matrix, wide chemical diversity of the metabolites and their wide concentration range, metabolite identification is intrinsically difficult. In our laboratory, we use automated mass spectral deconvolution and identification system (AMDIS) for identification of unknown VOMs. AMDIS first deconvolutes the raw GC-MS data file to find all components, and then compare mass spectral data against a library of target compound (e.g. National Institute of Standards (NIST) mass spectral library). To reduce possible solutions of identification offered by NIST Kovats retention index (RI) is used. A Kovats retention index system uses a series of standards, homologous series of n-alkanes applied as reference peak. Despite some limitations, presented methods could be very useful in VOMs identification. To confirm identification of unknown VOMs unequivocally, analysis of available analytical standards using the same GC-MS conditions is recommended.

Keywords: metabolomics, HS-SPME, AMDIS, Kovats retention index, NIST

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Identification of Synthetic Cannabinoid MMB CHMICA in "Spice-like" Herbal Mixture: Update of the Serbian Situation for the October 2017

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Synthetic cannabinoids, which were synthesized to improve the therapeutic effects of cannabis, have become a major issue when they are abused. They have different chemical structures from tetrahydrocannabinol (THC) but similar effects on endocannabinoid receptors. "Spice" named products have more serious side effects than cannabis and can even cause death. These mixtures are prepared by spraying chemicals onto small pieces of herbs and are being dishonestly sold as "natural" and "legal" products over the internet. Their popularity is continuously increasing. Although,