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HPLC-MS PHYTOCHEMICAL PROFILING AND DATABASE DEVELOPMENT FOR AUTHENTICATION OF MEDICINAL PLANTS USED IN DIETARY SUPPLEMENTS

Background/Aim. Recent amendments to the Ukrainian regulatory framework for dietary supplements have increased the need for reliable authentication and quality assessment of plant-derived ingredients. The aim of this study was to develop an HPLC-MS-based workflow and reference phytochemical database for authentication of medicinal plants and characterization of their bioactive constituents. **Methods.** More than 35 medicinal plant species traditionally used in Ukraine were collected and analyzed, while additional species continue to be investigated. HPLC-MS fingerprinting, phytochemical annotation, literature data analysis, and machine-learning-based prediction of biological activity were integrated into a unified workflow. **Results.** Characteristic HPLC-MS fingerprints were obtained for medicinal plant species and used to establish reference phytochemical profiles. Major chromatographic peaks and mass spectral features were annotated using published data and chemical databases. Particular attention was given to flavonoids, phenolic acids, terpenoids, and other compounds associated with reported biological activities. Machine learning models trained on publicly available bioactivity datasets were applied for preliminary *in silico* evaluation of identified phytochemicals. This approach enabled prioritization of compounds for further investigation and identification of metabolites with potential biological activity. The resulting database integrates botanical information, phytochemical composition, HPLC-MS fingerprints, literature-derived biological activities, and computational predictions. In addition, a comparative fingerprinting algorithm was implemented to assess similarity between chromatographic profiles and reference patterns, enabling rapid authentication of plant materials and detection of potential inconsistencies in raw botanical ingredients. **Conclusions.** The proposed workflow combines HPLC-MS phytochemical profiling, database development, and computational bioactivity assessment for systematic investigation of medicinal plants. The resulting database may serve as a valuable tool for authentication of botanical materials, characterization of bioactive compounds, and support of quality control procedures for plant-derived ingredients used in dietary supplements.

Keywords: medicinal plants, dietary supplements, HPLC-MS, phytochemical profiling, plant authentication, bioactive compounds, machine learning.

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