

AGASTACHE MEXICANA (LAMIACEAE) AS A MODEL FOR STUDY OF PLANT SECONDARY METABOLISM BY THE METABOLOMIC METHODS

© E. R. Kotlova,^{*,1,2} R. K. Puzanskij,^{**,1,2} T. Yu. Danchul,¹ L. I. Shagova,¹ I. A. Pautova,¹ A. L. Shavarda^{1,2}

¹ Komarov Botanical Institute of the Russian Academy of Sciences, St. Petersburg, Russia

² St. Petersburg State University, Russia

*E-mail: kotlova@yandex.ru

**E-mail: puzansky@yandex.ru

SUMMARY

Metabolite profiles of the chloroform, methanol and aqueous-ethanol extracts derived from vegetative (leaf) and reproductive (inflorescences and seeds) organs of the essential oil plant *Agastache mexicana* (Kunth) Lint et Epling, introduced in the nursery garden of BIN RAS, were comparatively analyzed by GC-MS. It was shown that above-ground organs of *A. mexicana* sampled at the phase of fruiting besides metabolites of primary metabolism such as free fatty acids, glycerolipids, organic acids, alcohols and sugars that are usually detected during metabolite profiling, accumulate significant amounts of secondary metabolites: sesqui- and triterpenoids, and phenolic compounds. To resolve the data structure revealed from the different plant organs and to unveil similarities and clustering of metaboloms, we used principal component analysis (PCA). PCA showed grouping samples into clusters in accordance with belonging to specific plant organs. Clear distinction between the clusters was also confirmed by the methods of classification: PLS-DA (Partial Least Squares Discriminant Analysis) and OPLS-DA (Orthogonal PLS-DA). Feature selection referring to difference between classes, extracted in line with inhering of sample to a particular organ of plant, allowed to identify a number of secondary metabolites with signs of organ specific allocation. Based on the data obtained we concluded that *A. mexicana* can be considered as a suitable model for studying secondary metabolism in plants, particularly terpenes and metabolically related steroids.

Key words: *Agastache mexicana*, metabolomics, multivariate analysis, secondary metabolism, sesquiterpenoids, triterpenoids, phytosterols.