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ORIGINAL PAPER

Exploratory chemometric grouping of fennel, anise, cumin, and coriander based on fatty acid composition

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Abstract

A data set of 17 specimens, five analysed in this study and 12 compiled from the literature (and therefore potentially affected by inter-laboratory analytical differences), yielded 26 fatty acids ranging from C4:0 to C24:0. The Ward's hierarchical clustering based on Semi-Partial R-Squared (SPR^2) distance metrics revealed compositional groupings among four Apiaceae spices: fennel (*Foeniculum vulgare*), anise (*Pimpinella anisum*), cumin (*Cuminum cyminum*), and coriander (*Coriandrum sativum*). Separate dendrograms were constructed for saturated and unsaturated fatty acids after mean-centering and unit-variance scaling. *Coriandrum sativum* showed the greatest compositional similarity among the evaluated coriander samples ($SPR^2 < 0.03$), supporting its potential use as a reference profile for quality assessment. Total C18:1 contents of 70.75-78.82% in coriander were consistent with the petroselinic-acid-rich chemotype reported in the literature; however, because routine GC-FID does not unambiguously resolve C18:1 positional isomers, these values should be interpreted as total C18:1 rather than definitive isomer-specific quantification. *Foeniculum vulgare* exhibited the widest intra-species variation: the Konya research sample was rich in C18:1 (75.14%), whereas the Diyarbakır sample was rich in linoleic acid (54.09% C18:2). C*uminum cyminum* displayed moderate compositional variation ($SPR^2 = 0.05$-0.10). Undecanoic acid (C11:0) was found at 3.2% and 6.5% in two coriander samples and only at a trace level (0.07%) in one fennel sample. It is therefore proposed as an exploratory candidate marker that requires targeted validation in a larger and more diverse sample set. The contrasting clustering patterns of saturated and unsaturated fatty acids are consistent with a hypothesis of partly independent regulation of fatty-acid biosynthesis, although no gene expression or enzyme activity data were collected. They also provide a preliminary quantitative basis for reference profiles in spice quality assessment. The observed variation also has nutritional and functional relevance, particularly because elevated myristic acid may adversely affect blood lipid profiles.

Keywords: Apiaceae, fatty acid profiling, hierarchical clustering, semi-partial R-squared

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