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AUTO-ML GC/MS FINGERPRINTING STRATEGY FOR CEREAL FLOUR AUTHENTICATION

***Kristian Pastor*[1], *Marko Ilić*[1], *Jovana Kojić*[2], *Nataša Nastić*[1], *Jelena Krulj*[2], *Marijana Ačanski*[1]**

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Despite food authentication being a global challenge since decades, not much work has been done in developing authentication methodologies of cereal flours and bakery products. This research represents an innovative and rapid method for classifying types of non-gluten and gluten-containing cereal flours: 10 corn, 5 wheat, and 5 barley samples. To achieve this aim, a gas chromatography – mass spectrometry (GC/MS) instrument was coupled to an automated machine learning algorithm (AutoML). Grains were sampled from the experimental fields of the Institute of Field and Vegetable Crops in Novi Sad, Serbia. Cereals were milled into flour, after which liposoluble matter was extracted with *n*-hexane, and derivatized into corresponding volatile compounds using a 0.2 M trimethylsulfonium hydroxide solution. Total ion current chromatograms consisting of 1666 datapoints/scans were used as raw signals, each of them representing a unique fingerprint of a cereal class. However, the aim of this work was to apply the Weka open-source software in automated mode, as a single, highly parametric machine learning framework for classifying types of flour into classes defined by botanical origin and gluten content. This was achieved using an Auto-Weka package with a state-of-the-art Bayesian optimization method, thus solving the combined algorithm selection and hyperparameter optimization (CASH) problem. The Weka's learning algorithm took into account all classifiers provided by the software: 27 base learners, 10 meta-methods, and 2 ensemble methods. Both 60 and 120 min time-budgets were carried out by the computer unattended. In each case, a Support Vector classifier (SMO) using normalized polynomial kernel was recommended as the most optimal, using a 10-fold cross-validation to exploit the performance gains on a given dataset. Cereal flour samples were adequately classified in 3 groups: non-gluten corn, and gluten wheat and barley. The presented approach directly supports the application of artificial intelligence on processing chemical information, in order to develop methods for food authentication.

Keywords: Authentication, Automated machine learning, Gas chromatography – mass spectrometry, Cereal flour, Classification

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