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Effect of Preprocessing High-Resolution Mass Spectra on the Pattern

Recognition of *Cannabis*, Hemp, and Liquor

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Abstract

High-resolution mass spectrometry (HRMS) combined with pattern recognition was used to discriminate among twenty-five *Cannabis* samples, twenty hemp samples, and eight liquor samples. The effects of preprocessing on multivariate data analysis were evaluated for Orbitrap high-resolution mass spectra. Different root transformations were evaluated with respect to the bin width and the average classification rates. In addition, linear binning and proportional binning with various resolving powers were studied with respect to the average classification rates. The proportional binning with the square root transformation gave the best overall performance for chemical profiling or spectral fingerprinting. Six classification methods, fuzzy rule-building expert system (FuRES), linear discriminant analysis (LDA), super partial least squares discriminant analysis (sPLS-DA), support vector

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