

Área: ANA

Low-Resolution CZE-MS screening data of urine samples associated with Machine Learning modeling for discriminative classification of COVID-19

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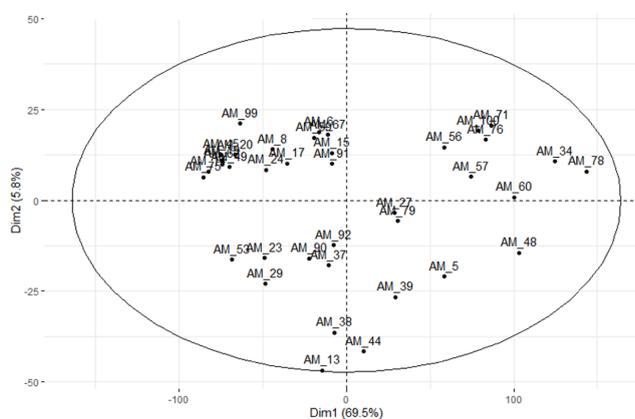
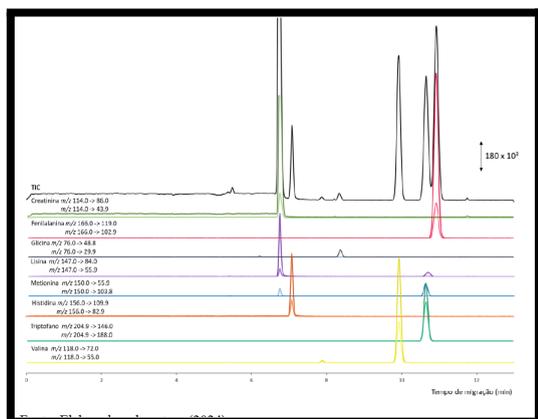
Palavras Chave: CZE-MS, Machine Learning, COVID-19

Highlights

A novel capillary electrophoresis and low-resolution MS approach combined with machine learning for distinguishing COVID-19 positive from negative cases from urine samples

Resumo/Abstract

Aiming at a focused study to detect low-weight cations resembling amino acid structures of key groups of biomarker candidates for COVID-19 diagnosis, a dataset containing low-resolution mass spectra information was collected using a CZE-QQQ system followed by machine learning processing. Since amino acids are fundamental components in human urine and are formed as end-products of metabolic pathways, an analytical method was developed based on the intrinsic selectivity of CZE combined with mass spectrometry. Urine samples from 100 volunteers who underwent RT-PCR testing for COVID-19 were analyzed. These samples were divided into a Test Group (38) and a Control Group (62) using an Agilent 7100 CE triple Quadrupole system, operated in ESI (+) mode with a m/z range from 20 to 500. CZE was performed with normal polarity in a pH 3 BGE with hydrodynamic injection. The raw mass spectra dataset was processed using a Random Forest algorithm, with a variable selection strategy focusing on m/z values differentiating positive and negative cases. The model achieved 80% accuracy and 0.612 MCC. Although it does not yet meet the accuracy standards for diagnostic applications, this study provides valuable insights into using capillary electrophoresis coupled with low-resolution MS for investigative metabolomics, offering crucial information for health-related issues and complex analytical environments.



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