Identification of Propionibacteria to the species level using Fourier transform infrared spectroscopy and artificial neural networks

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Abstract

Fourier transform infrared spectroscopy (FTIR) and artificial neural networks (ANN’s) were used to identify species of Propionibacteria strains. The aim of the study was to improve the methodology to identify species of Propionibacteria strains, in which the differentiation index D, calculated based on Pearson’s correlation and cluster analyses were used to describe the correlation between the Fourier transform infrared spectra and bacteria as molecular systems brought unsatisfactory results. More advanced statistical methods of identification of the FTIR spectra with application of artificial neural networks (ANN’s) were used. In this experiment, the FTIR spectra of Propionibacteria strains stored in the library were used to develop artificial neural networks for their identification. Several multilayer perceptrons (MLP) and probabilistic neural networks (PNN) were tested. The practical value of selected artificial neural networks was assessed based on identification results of spectra of 9 reference strains and 28 isolates. To verify results of isolates identification, the PCR based method with the pairs of species-specific primers was used.

The use of artificial neural networks in FTIR spectral analyses as the most advanced chemometric method supported correct identification of 93% bacteria of the genus Propionibacterium to the species level.

Key words: Propionibacteria, FTIR spectra, PCR, artificial neural networks

Introduction

Microbial diversity results from variations in bacteria’s morphological and biochemical characteristics. Bacterial Fourier transform infrared (FTIR) spectra are strain-specific, and they demonstrate the characteristic features of the strain’s cellular components such as fatty acids, membrane proteins, intracellular proteins, polysaccharides and nucleic acids (Naumann et al. 1991b, Schmitt et al. 1998). The spectra of intact bacterial cells are a specific representation of the studied cell’s phenotypic and genotypic properties. Naumann et al. (1991a) proposed to analyze bacterial FTIR spectra as dactyloscopic images. The differences between various microbial spectra are difficult to observe, which is why they have to be analyzed with the use of statistical methods. The most popular statistical techniques (Mariey et al. 2001,