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ePoster Viewing
Diagnostic bacteriology – non-culture based, including molecular and MALDI-TOF

A novel genetic algorithm for Maldi-ToF mass spectrometry based identification of bacterial species

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Background: An original genetic algorithm for identification of bacterial species using MALDI mass spectra and genomic information was developed. The algorithm is based on the abundance statistics of ribosomal and other high-represented proteins in MALDI mass spectra and the database of bacterial genomes containing information for more than 4000 species. The algorithm compares m/z values of MALDI mass-peaks of a given organism and a set of theoretical m/z values of ribosomal and other proteins from the database. The probability of a match between an unidentified species with known MALDI mass spectrum and a species from the genomic database is predicted by a scoring function.

This study was aimed to verify this new genetic algorithm for identification of bacterial species in laboratory setting.

Material/methods: A total of 507 bacterial isolates belonged to 54 different species were involved. They were represented by clinically relevant microorganisms such as Enterobacteriaceae, non-fermenting Gram-negative bacilli, and Gram-positive cocci. The raw bacterial MALDI mass spectra were obtained using an Autoflex LT (Bruker Daltonics, Germany) mass spectrometer and analysed by MALDI Biotyper 3.1 (Bruker Daltonics, Germany) for species identification. Further these spectra were analyzed using the developed genetic algorithm. Additionally, mass spectra for same bacteria were collected using a LaserToF TT (SAI, UK) mass spectrometer and tested via the genetic algorithm for species identification.

Results: All of bacterial isolates were identified by both Biotyper 3.1 and the genetic algorithm with suitable score. In case of “bruker’s” mass spectra the genetic algorithm correctly identified 95.9% (486/507) isolates to species level and 98.6 % (500/507) to genus level.

The analysis of SAI mass spectra by the genetic algorithm resulted in the identical species identification in 94.1% (477/507) cases and in 98.2 % (498/507) there were matches at the genus level. The most common mismatches were *Klebsiella oxytoca* vs *Raoultella ornithinolytica*, and *Stenotrophomonas maltophilia* vs *Pseudomonas geniculata*. It can be explained by constant changes in modern taxonomy of bacterial species or probable mixed bacterial culture.

Conclusions: The genetic algorithm demonstrated high sensitivity and specificity for bacterial species identification regarding to Biotyper 3.1 (Bruker Daltonics, Germany), but in contrast to the latter one could be successfully used with different MALDI ToF mass spectrometry platforms.

Unlike actual commercial solution for mass spectrometry identification using referential proteomic profiles, the presented approach is based on bacterial genomes, which amount extents exponentially, so the genetic algorithm seems to be more flexible and informative. Consequently the genetic algorithm is supposed to be a promising method for rapid typing of closely related species, identifying serotypes and pathogenic strains.