MALDI-TOF mass spectrometry for typing

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Mass spectrometric analysis of bacterial raw extracts has revolutionised microbiology in the recent years. Analysis by matrix-assisted laser desorption/ionisation time-of-flight mass spectrometry (MALDI-TOF MS) for this purpose is rapid and economic, the resulting spectra can be very informative. These extraordinary features for the identification of bacteria have lead to the extension of the approach for the characterisation of other microorganisms like yeasts or fungi, and also of tissue cultures and whole animals, especially arthropods. The interest of many users focuses on the question of how detailed MALDI-typing can be at best. Concerning bacteria, it is of greatest interest to which taxonomic level samples can be classified and, in a number of cases, if biovars or serotypes can be reliably distinguished. In contrast to the identification of proteins or peptides by mass spectrometry, the identification of the analyte by MALDI-typing is not based on the comparison of the experimental spectrum with masses calculated from a sequence database but rather on the comparison of the analyte spectrum with a library of reference spectra from authentic samples. Although widely applied, some theoretical aspects of mass spectrum-based classification have not been fully addressed yet. A number of commercial and in-house softwares implementing different classification algorithms are in use, complicating cross-platform comparison of typing results. One step in most algorithms used for classification is data reduction, i.e. the selection of masses from the reference or sample spectra that are useful for classification. This is especially necessary for the distinction of closely related organisms like subspecies or serotypes, as their spectra will only present a limited number of differing masses. In an effort to characterise the spatial and temporal distribution of Shiga toxin-producing Escherichia coli (STEC) isolates representing the serotypes O165:H25, O26:H11/H32, and O156:H25, we have analysed MALDI-type spectra by systematic variation of the data reduction step in our classification algorithm. With optimised parameters, the classification of all three O-serotypes was possible with a false rate below 1%. For all combinations of two of the three groups, parameters could be adjusted to accurately distinguish the two groups.