SHIMADZU
Excellence in Science

MO347

Microorganism Identification and Molecular Profiling Using MALDI-TOF-MS

iD*plus*

iD*plus*™ - Take Analysis Further

iD*plus*

- Rapid microbial identification for research use
- Identifies and classifies strains based on phenotype characteristics
- SuperSpectra™ reduce the incidence of false positives and ensure robustness and reproducibility
- Open system allows addition of new species / entries to the database or the creation of new databases
- Clustering allows molecular profiling and tracking of change or evolution
- High performance MS for large molecule analysis
- MS/MS options allow structural analysis

MALDI-TOF

Matrix Assisted Laser Desorption / Ionization Time-of-Flight Mass Spectrometry

The biomolecules embedded in the matrix crystals are desorbed and ionized by a laser pulse and accelerated in a high voltage field. Different ions are detected after a time-of-flight proportional to their mass, generating a high resolution mass spectrum of the sample: the 'profile'.

Depending on the choice of mass spectrometer, both intact large molecules (linear mode) and structural determination of fragments (reflectron mode) can be investigated.

iD*plus* Platform Portfolio: A Complete Range to Suit All Needs

iD*plus* Assurance
Linear MALDI-TOF

System for simple microbial identification using SARAMIS™ and basic analytical life sciences using LaunchPad™. Combining speed of analysis, positive and negative ionization and wide mass range, the iD*plus* Assurance provides excellent quality and reliability in a general analytical setting.

iD*plus* Confidence
Reflectron MALDI-TOF

The patented curved-field reflectron design in the iD*plus* Confidence extends analysis possibilities beyond simple identification. Expanding on microbial ID, reflectron mode ensures the high resolution and high mass accuracy required for molecular profiling and structural analysis.

iD*plus* Performance
MALDI TOF-TOF

Delivers flexibility and ease of use in a robust and reliable research-grade instrument. Advanced MS/MS performance utilizing the highest collision energy to fragment compounds for accurate structural analysis.

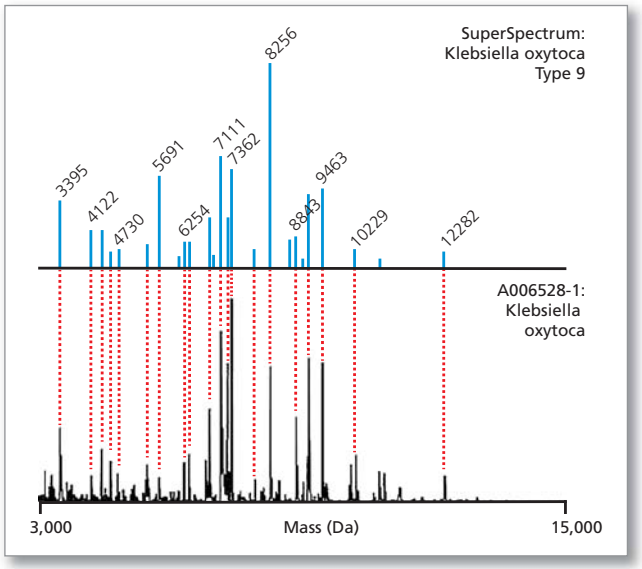
The most versatile iD*plus* platform from simple identification to in-depth proteomics, lipidomics and sequencing.

iD*plus*: Simple, Fast, Effective Identification of Microorganisms

iD*plus* utilizes SARAMIS: the easy to use microbial identification software which has revolutionized daily routine in analytical and diagnostic-research laboratories. It comprises one of the AXIMA™ MALDI-TOF mass spectrometers and the SARAMIS database (Spectral ARchive And Microbial Identification System).

MALDI-TOF mass spectra of bacteria and fungi are highly taxon-specific and can be used for specimen identification. The SARAMIS database includes both SuperSpectra and reference spectra which have been derived from the MALDI analysis of isolates identified by widely accepted methods such as phenotyping, 16sRNA analysis or MLST (Multi-Locus Sequence Typing).

Each SuperSpectrum is derived from multiple reference spectra (mass profiles) of at least eight individual isolates of a species (on average), acquired after varying growth times and from different growth media to ensure robustness and reproducibility.



SARAMIS offers a comprehensive database of species (supported by internationally recognized strain collections and clinical laboratories) and the flexibility for the user to create new entries and databases.

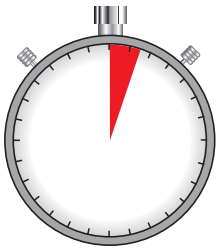
Cultured microorganisms can be directly applied to the MALDI sample target and introduced into one of the iD*plus* series mass spectrometers. Analysis and identification can be completed in 1-2 minutes.

The software identifies gram-positive and gram-negative bacteria, yeasts, fungi and algae based on their characteristic MALDI-TOF-MS profiles down to sub-species level. No preselection of analytical methods is required; hands-on time is reduced and costs are cut dramatically.

From Unknown to Identification in Two Simple Steps

Step 1: Preparation

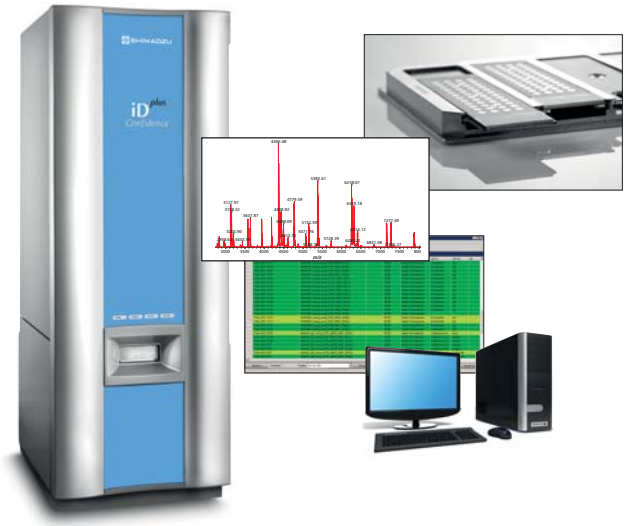
iD*plus* identifies a sample grown overnight on a culture plate. A small number of cells is transferred to a FlexiMass-DS™ disposable polymeric target, followed by the addition of a matrix solution. The sample is then air-dried.



Just 2-3 minutes for sample transfer and identification.

Step 2: Identification

The FlexiMass-DS target is loaded into the MALDI-TOF where the mass spectral profiles of the samples are acquired. These profiles are matched against the SARAMIS database of SuperSpectra for immediate identification. Results are displayed within 1-2 minutes.



Dedicated Software Solutions

Target Manager and Automated Identification

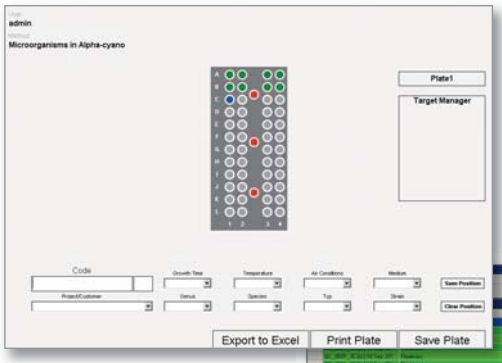
Dedicated Target Manager software ensures that all the relevant sample information (e.g. growth time, temperature, environment and medium) is associated directly with the sample. For each sample, Target Manager highlights the plate location for sample deposition and associates the acquisition method and parameters with each sample. This is then transferred to the MALDI for data acquisition simplifying the iD*plus* workflow.

The sample mass spectrum is automatically processed and condensed to a profile peak list containing the mass / intensity data. This is then searched against the SuperSpectra in the SARAMIS database. iD*plus* typically identifies 95% of clinical samples unambiguously within one minute.

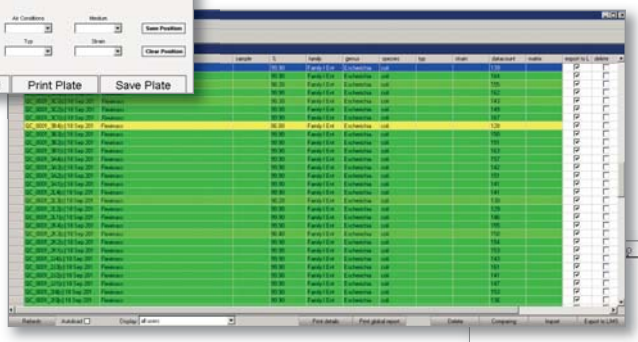
In uncertain cases, when the identification confidence is below 90%, the sample profile is re-searched against all available reference spectra in the database collected since 1998 – a significant improvement for the identification of atypical specimens.

Patented identification procedures are designed to prevent false identifications by setting stringent thresholds for significant database matches.

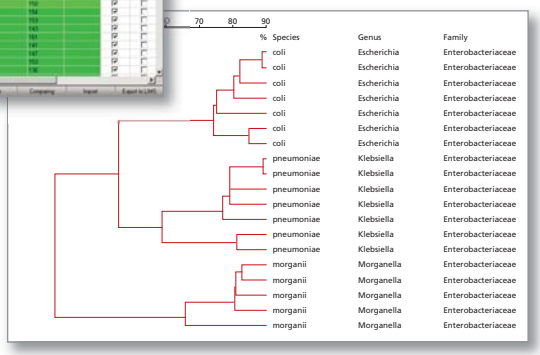
Manual acquisition is also possible when fewer samples are being analyzed or greater control is required.



Target Manager software



Microbial identification result



Hierarchical cluster analysis

Hierarchical Clustering

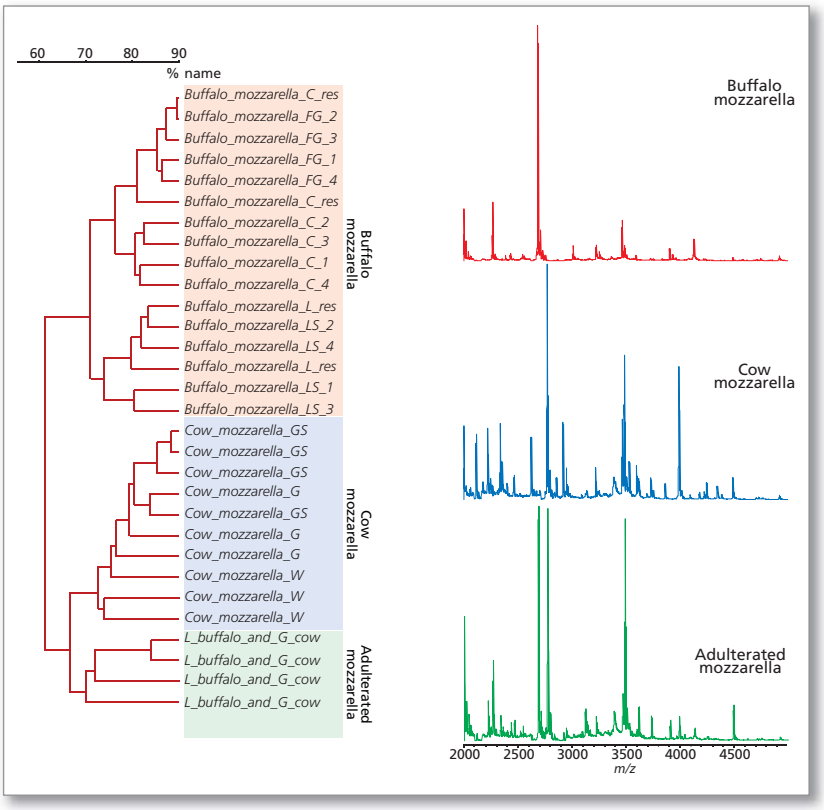
The SARAMIS software is able to carry out hierarchical clustering of samples, the results being represented by dendrograms. This technique can be used to identify changes in the sample population over time, or to create new SuperSpectra which are representative of a particular environment.

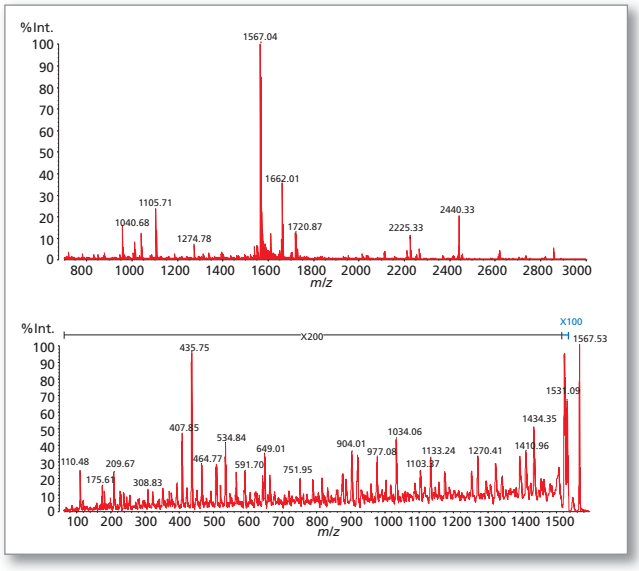
iD*plus* - Take Analysis Further™

Molecular Profiling: Food Adulteration

The flexibility of the open database associated with iD*plus* allows the use of the platform for molecular profiling experiments and differentiation of related samples based on the unique features in their profile. New custom sample-specific entries (SuperSpectra) can be added to create a sub-database relevant to a particular area of research. This has been reported in areas as diverse as entomology, zooplankton research, eukaryotic cells, fish speciation and the study of food-borne bacteria. Molecular profiling is also an effective technique in the analysis of adulterated foodstuffs.

The example shown (*right*) is that of food adulteration in the dairy industry. The iD*plus* molecular profiles for cow, buffalo and adulterated mozzarella show significant differences. Cluster analysis in SARAMIS resulted in three distinct groups corresponding to the cow, buffalo and adulterated mozzarella.





Proteomics: Resistance Markers

Extended spectrum β-lactamases (ESBLs) confer resistance to a wide spectrum of β-lactam antibiotics severely limiting antibiotic treatment options. Detection of specific resistance markers indicative of ESBLs in laboratory isolates (varied plasmid constructs) was achieved using a combination of the iD*plus* platform and LC-MALDI analysis. Three laboratory *E. coli* isolates exhibiting different β-lactamase resistance mechanisms (TEM, CTX-M15 and KanR) were analyzed. MS/MS peptide sequencing carried out on tryptic digests of extracts from the isolates revealed several biomarkers indicative of each resistance mechanism.

Examples of MS and MS/MS data from one of these isolates are shown. Mascot database search results for the whole dataset identified an enzyme linked to CTX-M type β-lactamase. This demonstrates the ability of the iD*plus* platform to discriminate at the species level and at an identical strain level where the only difference between the strains is the carriage of a modified antibiotic resistance carrying plasmid.

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SHIMADZU

Kratos Analytical Ltd.
Wharfside, Trafford Wharf Road, Manchester M17 1GP, UK
Phone: +44 161 888 4400 Fax: +44 161 888 4402
URL http://www.shimadzu.com/an/

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