MASsoft Professional

• An overview of new features including:
  • Automatic peak identification and spectral analysis
  • 3D data plots
Windows® MASsoft Professional PC software new features

Three new key features:

• Automated spectral analysis providing peak identification and composition analysis.

• Spectral simulation mode to compare predicted analysis spectrum with the recorded spectrum.

• 3D data plot for viewing mass vs. electron energy intensity.
Automatic peak identification and automatic analysis

Tools for analysis include:

- Library groups edited and selected to be appropriate for the application.
- Peak identification – colour coded to indicate library match.
- Spectral simulation and subtraction tools providing difference spectra for comparison to recorded data.
- Parameter control to set thresholds for peak inclusion.
Users select and edit library groups to match the analysis application. Default library groups include:

Library groups – enables application specific peak identification
Scan example sampling air

Peak identification and Auto Analysis functions
The automatic peak identification finds the air peaks
Peak identification and automatic analysis:

MASsoft includes predictive genetic algorithms to evaluate spectra, identify species present and calculate the gas composition.

The software includes user adjustable parameters to enhance the match including:

- Number of peaks matched.
- Ignore small peaks to reduce large number of hits.
- Scaled peak intensity.

Recorded, predicted and difference spectra
Complex example.
The automatic peak identification finds and identifies the possible species.
The report includes:

Species with % composition.

Identified peaks in the recorded data.

Stacked peaks in graph/table.

Accuracy of the analysis. The mean square error value is reported. This is a confidence factor for the accuracy of the analysis.

The analysis report is exported as a PDF.
The new 3D data view allows users to view multi-variant scans in 3D. Multi-variant parameters include: mass, electron energy, focus and other ion optical lenses.
3D data - Argon mass 20 vs electron energy
APSI - MS appearance potential soft ionisation mass spectrometry
3D View of Argon mass 20 vs electron energy

APSI-MS: Appearance Potential Soft Ionisation Mass Spectrometry
3D View of Argon mass 20 vs electron energy - rotated

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