

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

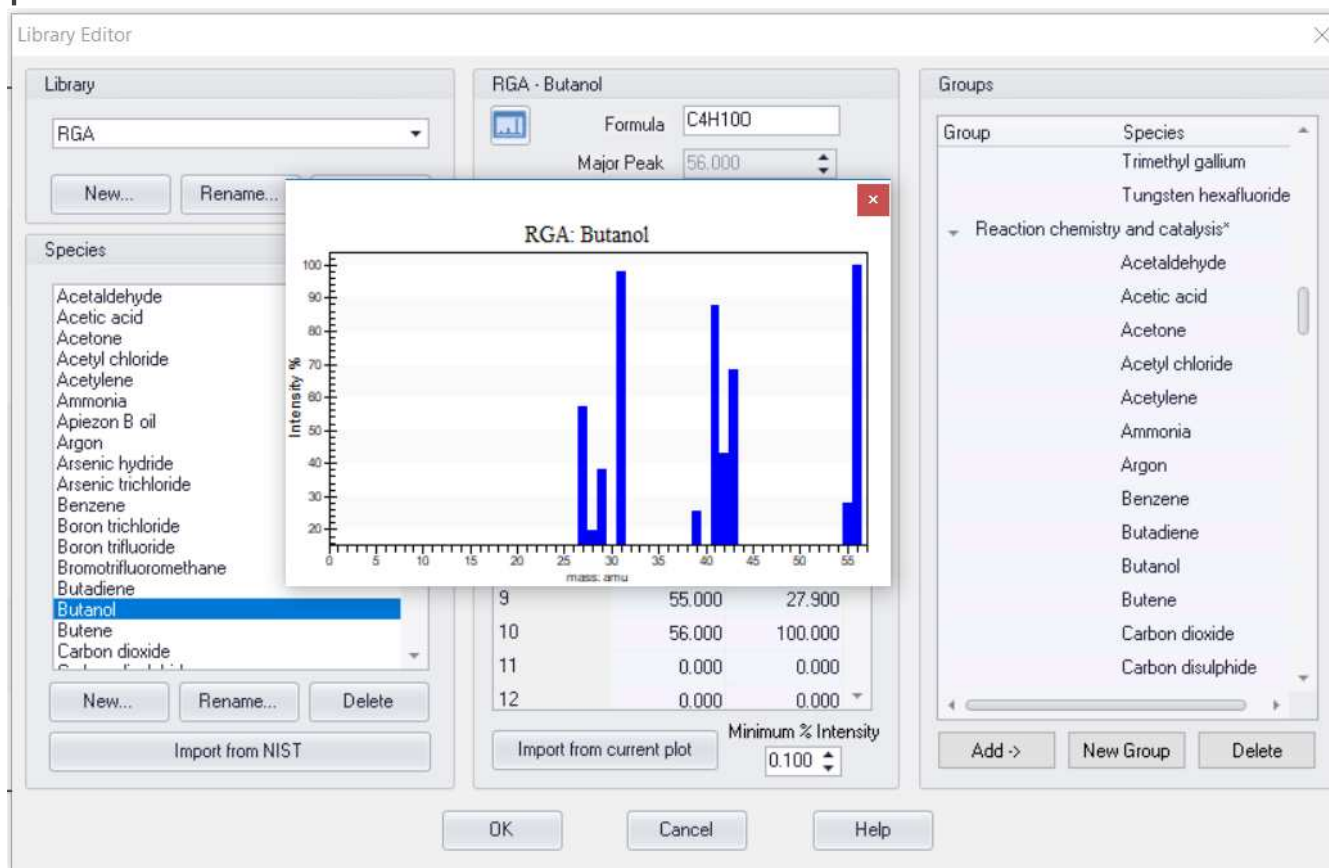
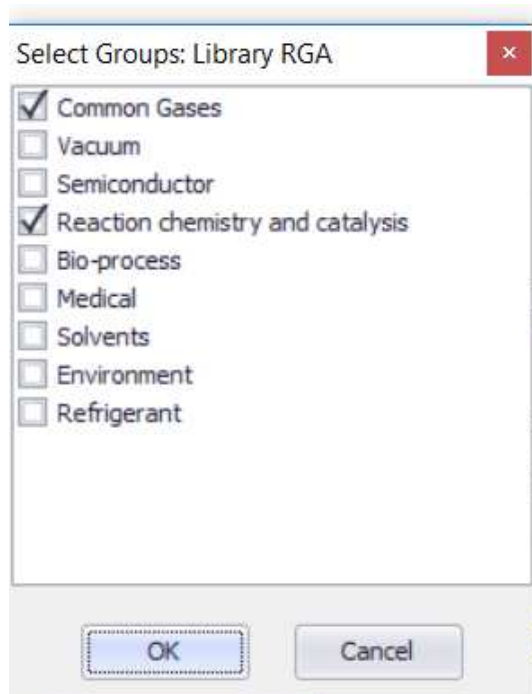
Tools for analysis include:

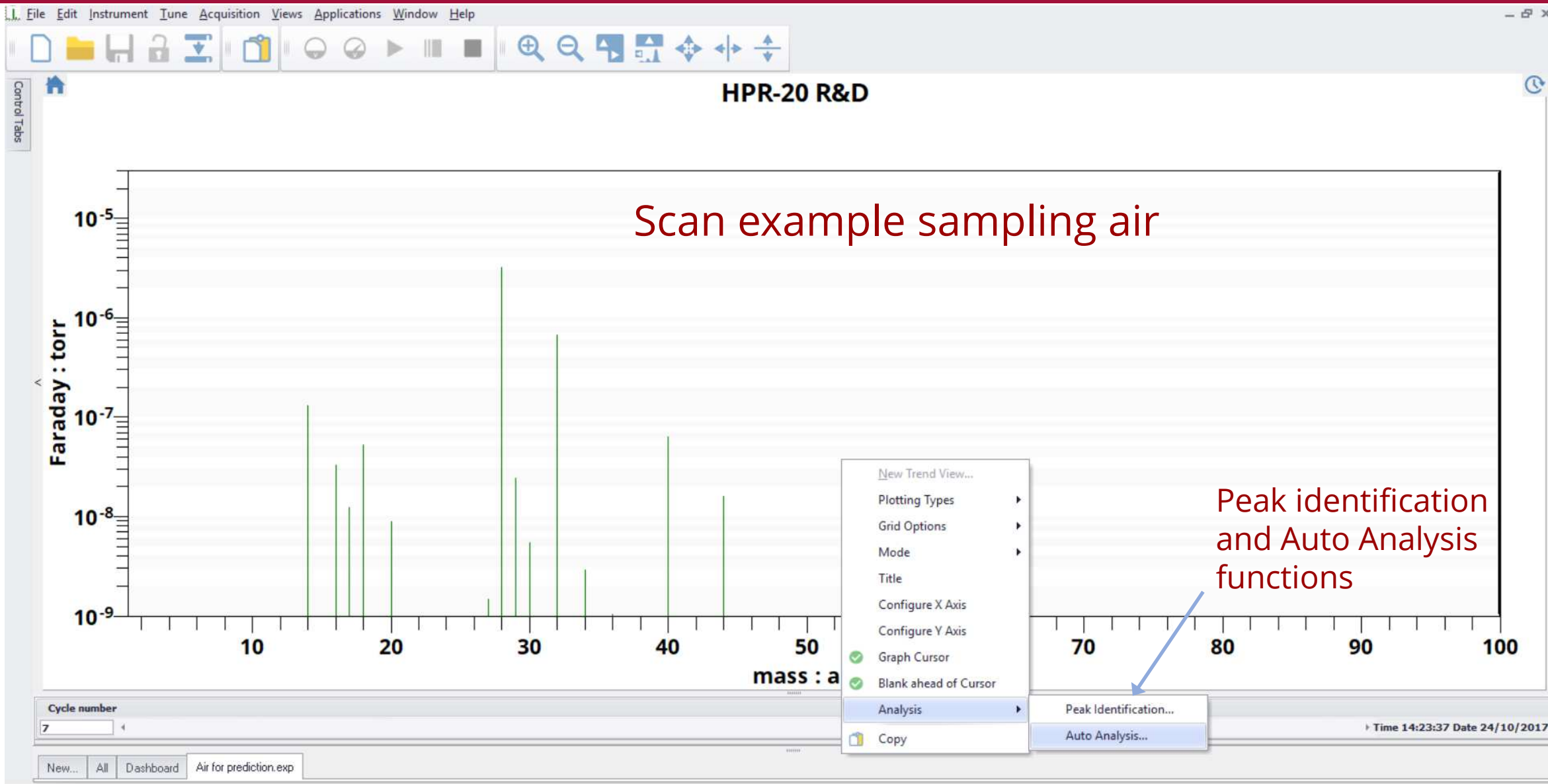
- Library groups edited and selected to be appropriate for the application.
- Peak identification – colour coded to indicate library match.
- Spectral simulation and subtraction tools providing difference spectra for comparison to recorded data.
- Parameter control to set thresholds for peak inclusion.

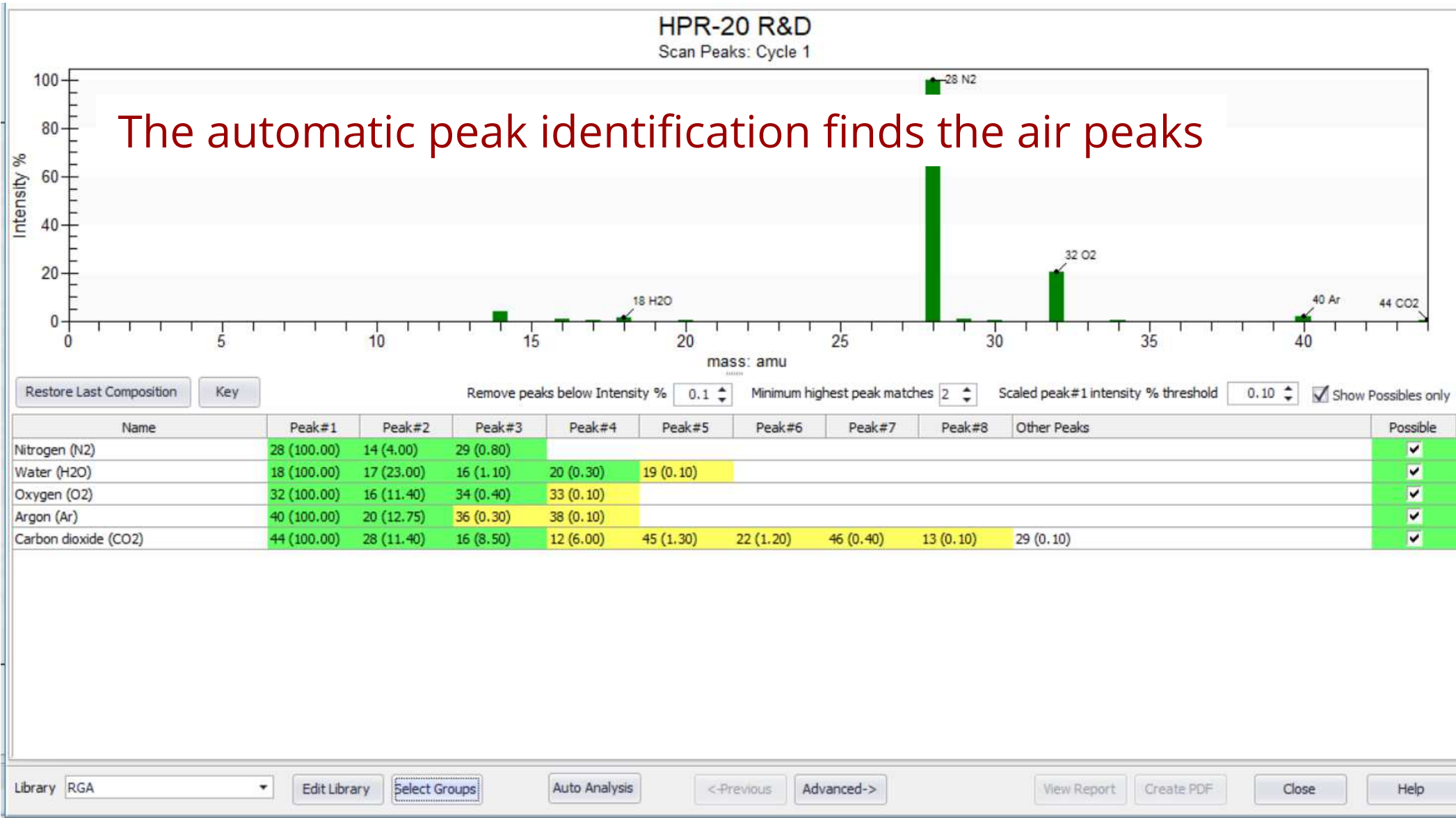
Library groups – enables application specific peak identification

Users select and edit library groups to match the analysis application.

Default library groups include:







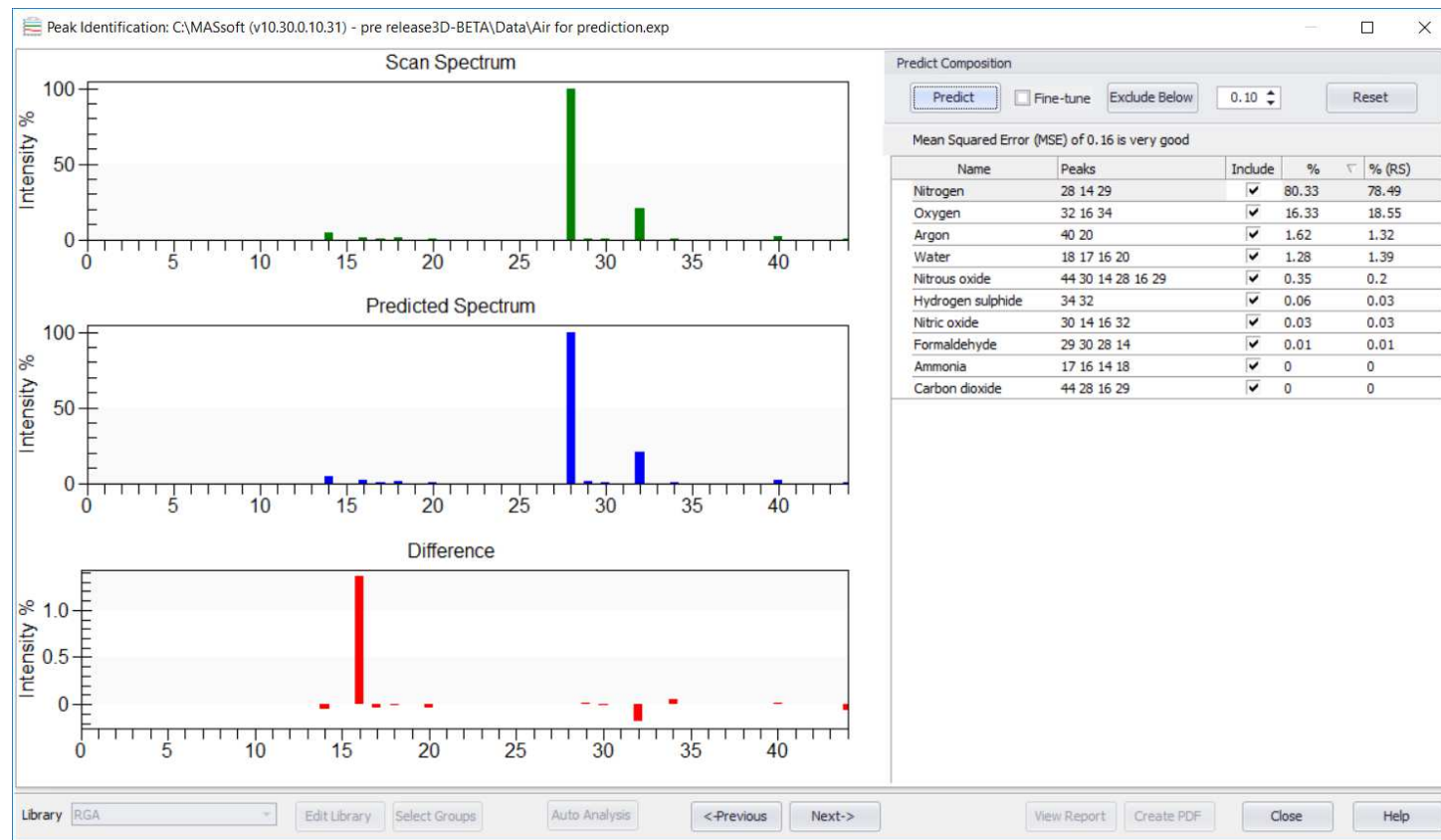
Recorded, predicted and difference spectra

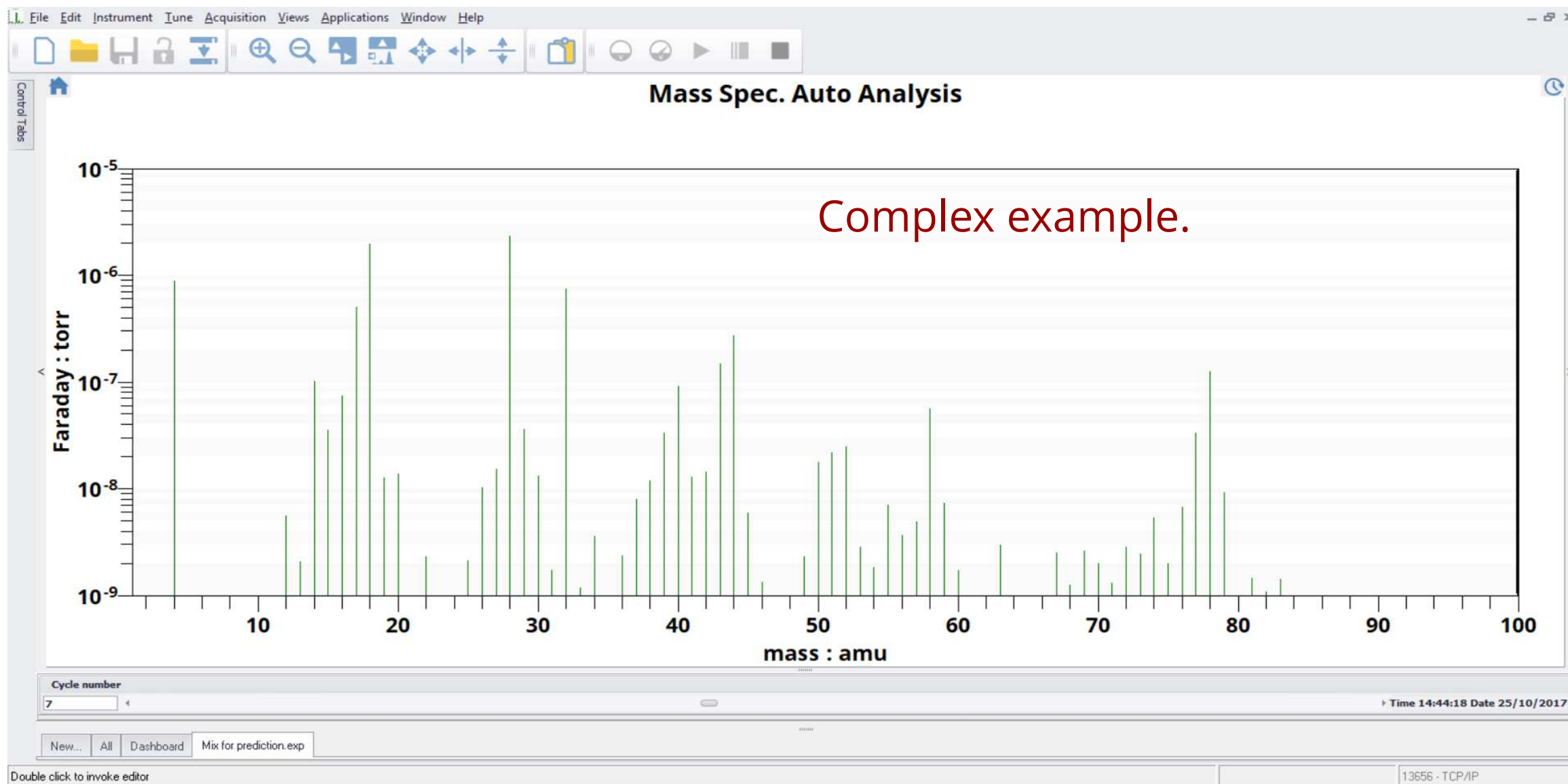
Peak identification and automatic analysis:

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:

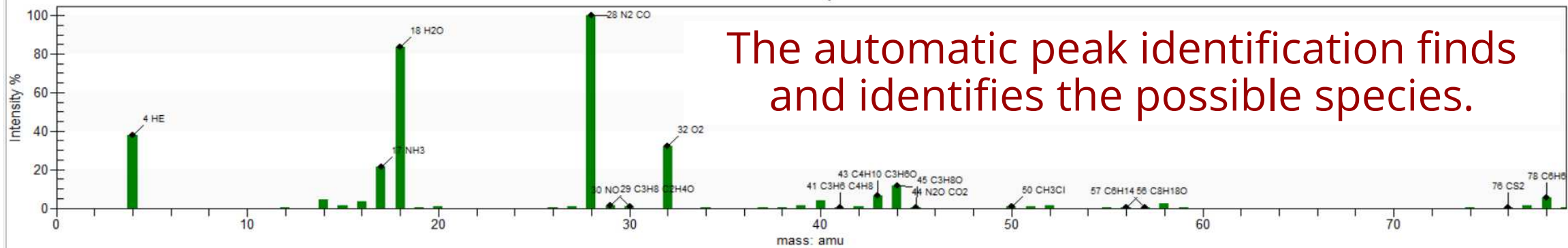
- Number of peaks matched.
- Ignore small peaks to reduce large number of hits.
- Scaled peak intensity.





Mass Spec. Auto Analysis

Scan Peaks: Cycle 7



Restore Last Composition

Key

Remove peaks below Intensity %

0.2

Minimum highest peak matches

3

Scaled peak#1 intensity % threshold

0.20

Name	Peak#1	Peak#2	Peak#3	Peak#4	Peak#5	Peak#6	Peak#7	Peak#8	Other Peaks	Possible
Propane (C3H8)	29 (100.00)	26 (76.00)	28 (59.10)	15 (39.00)	27 (37.90)	44 (26.20)	14 (25.00)	43 (22.30)	39 (16.20) 41 (12.40) 42 (5.10) 38 (4.90) 37 (3.10) 40 (2.80) 30 (2.10) 45 (0.10)	✓
N-Butane (C4H10)	43 (100.00)	29 (44.20)	27 (37.10)	28 (32.60)	41 (27.80)	39 (12.50)	42 (12.50)	58 (12.30)	26 (6.20) 15 (5.30)	✓
Acetone (C3H6O)	43 (100.00)	58 (27.10)	27 (8.00)	42 (7.00)	26 (5.80)	29 (4.30)	39 (3.80)	38 (2.30)	37 (2.10) 41 (2.10)	✓
Propene (C3H6)	41 (100.00)	39 (74.00)	42 (69.60)	27 (38.40)	40 (29.00)	38 (20.30)	37 (13.40)	26 (11.30)	15 (5.90) 14 (3.90)	✓
Carbon disulphide (CS2)	76 (100.00)	32 (21.80)	44 (17.30)	78 (8.90)	38 (6.40)	28 (5.40)	77 (2.60)	14 (1.00)	34 (1.00)	✓
Butene (C4H8)	41 (100.00)	56 (38.80)	39 (33.90)	28 (27.00)	27 (25.10)	55 (18.10)	29 (12.50)	26 (8.20)	40 (6.40) 53 (5.40)	✓
Hexane (C6H14)	57 (100.00)	43 (81.20)	41 (70.10)	29 (60.60)	27 (45.40)	56 (45.30)	42 (40.90)	39 (19.70)	86 (15.50) 28 (10.70)	✓
Isopropyl alcohol (C3H8O)	45 (100.00)	43 (16.60)	27 (15.70)	29 (10.10)	19 (6.60)	41 (6.60)	39 (5.70)	31 (5.60)	42 (4.00) 59 (3.40)	✓
Nitrogen (N2)	28 (100.00)	14 (4.94)	29 (0.73)							✓
Carbon monoxide (CO)	28 (100.00)	12 (4.50)	29 (1.10)	16 (0.90)	14 (0.60)	30 (0.20)				✓
Helium (HE)	4 (100.00)									✓
Water (H2O)	18 (100.00)	17 (23.00)	16 (1.10)	20 (0.30)	19 (0.10)					✓
Benzene (C6H6)	78 (100.00)	52 (19.40)	51 (18.60)	50 (15.70)	77 (14.40)	39 (14.20)	38 (5.80)			✓
Ammonia (NH3)	17 (100.00)	16 (80.00)	15 (7.50)	14 (2.20)	18 (0.40)					✓
Nitrous oxide (N2O)	44 (100.00)	30 (31.10)	14 (12.90)	28 (10.80)	16 (5.00)	45 (0.70)	46 (0.20)	15 (0.10)	29 (0.10) 31 (0.10)	✓
Acetaldehyde (C2H4O)	29 (100.00)	44 (45.70)	43 (26.70)	42 (9.20)	26 (9.10)	25 (4.80)	27 (4.50)	41 (3.90)	28 (2.70) 24 (1.60)	✓
Nitric oxide (NO)	30 (100.00)	14 (7.50)	15 (2.40)	16 (1.50)	31 (0.40)	32 (0.20)				✓
Oxygen (O2)	32 (100.00)	16 (11.40)	34 (0.40)	33 (0.10)						✓
Octanol (C8H18O)	56 (100.00)	55 (87.50)	41 (80.70)	43 (74.90)	70 (61.00)	69 (58.60)	42 (56.30)	84 (48.70)	57 (38.50) 29 (34.80)	✓
Carbon dioxide (CO2)	44 (100.00)	28 (11.40)	16 (8.50)	12 (6.00)	45 (1.30)	22 (1.20)	46 (0.40)	13 (0.10)	29 (0.10)	✓
Methyl chloride (CH3Cl)	50 (100.00)	15 (72.30)	52 (31.00)	49 (11.40)	14 (8.40)	47 (7.10)	35 (6.20)	13 (5.40)	51 (3.80) 48 (3.40)	✓
Pentane (C5H12)	43 (100.00)	42 (61.10)	41 (57.50)	57 (19.90)	39 (19.30)	27 (18.90)	29 (13.60)	72 (12.90)	55 (5.40) 56 (4.10)	✓

Library RGA

Edit Library

Select Groups

Auto Analysis

<Previous

Advanced->

View Report

Create PDF

Close

Help

Analysis Report - PDF

The report includes:

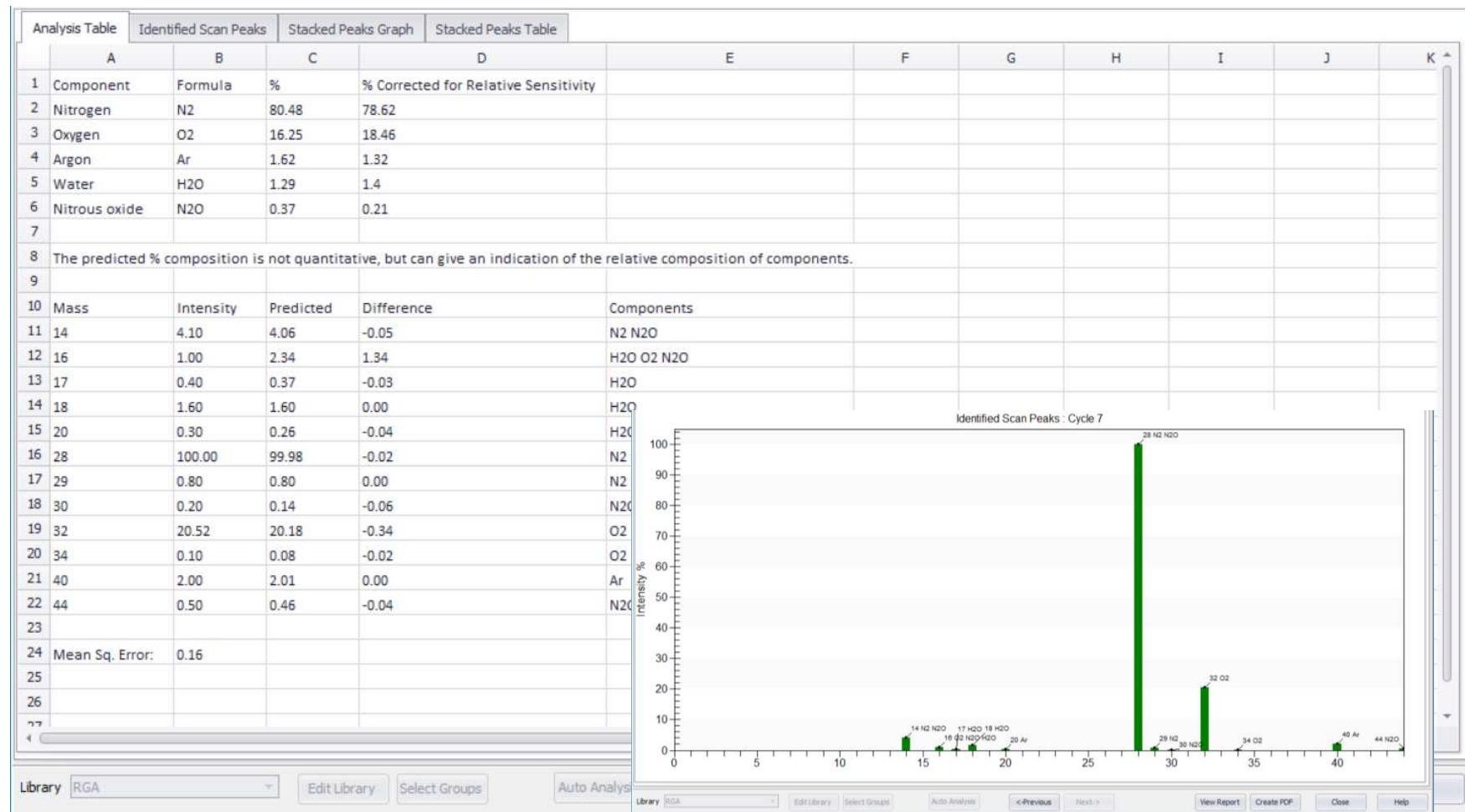
Species with % composition.

Identified peaks in the recorded data.

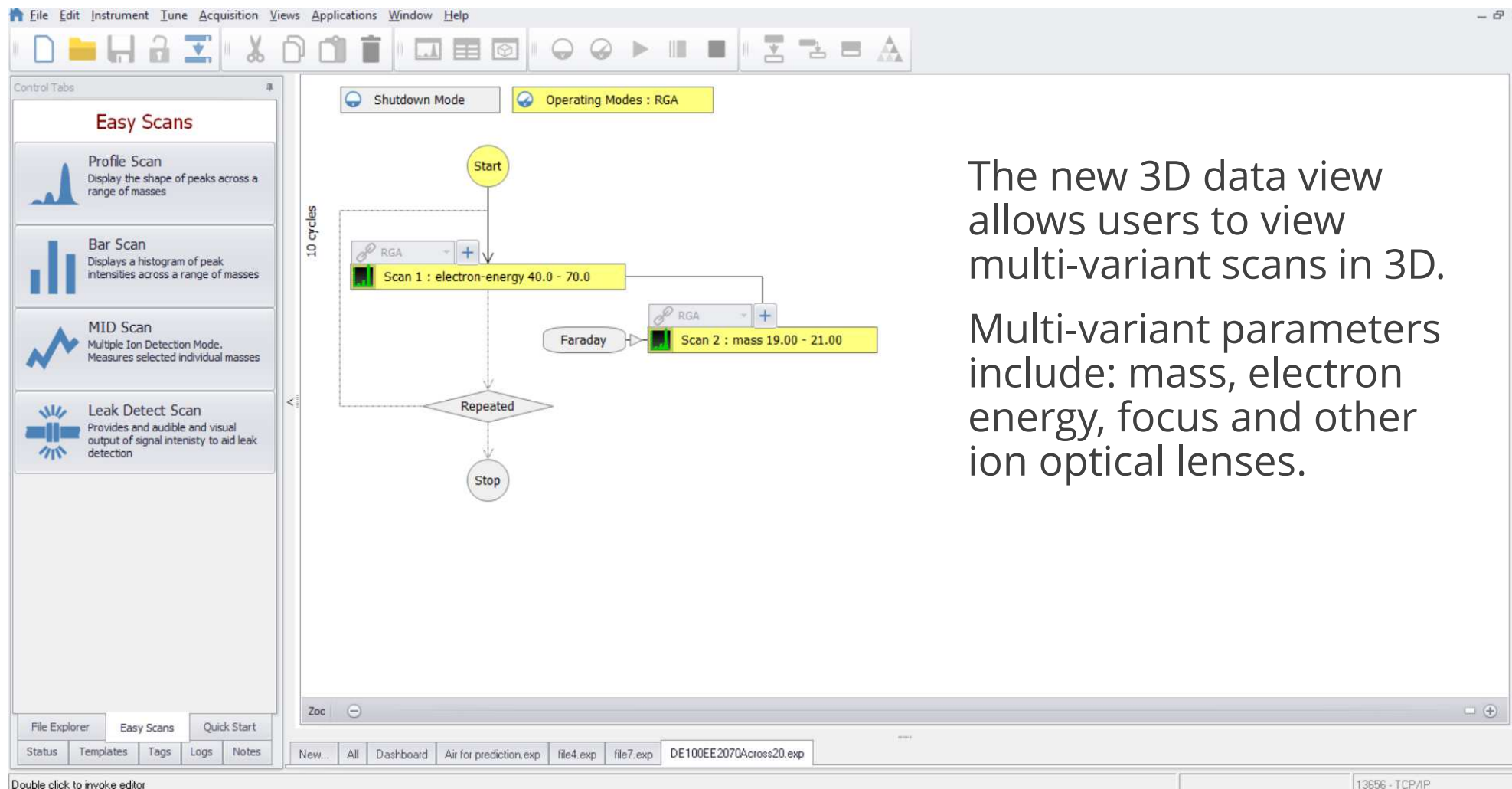
Stacked peaks in graph/table.

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.



3D Data View

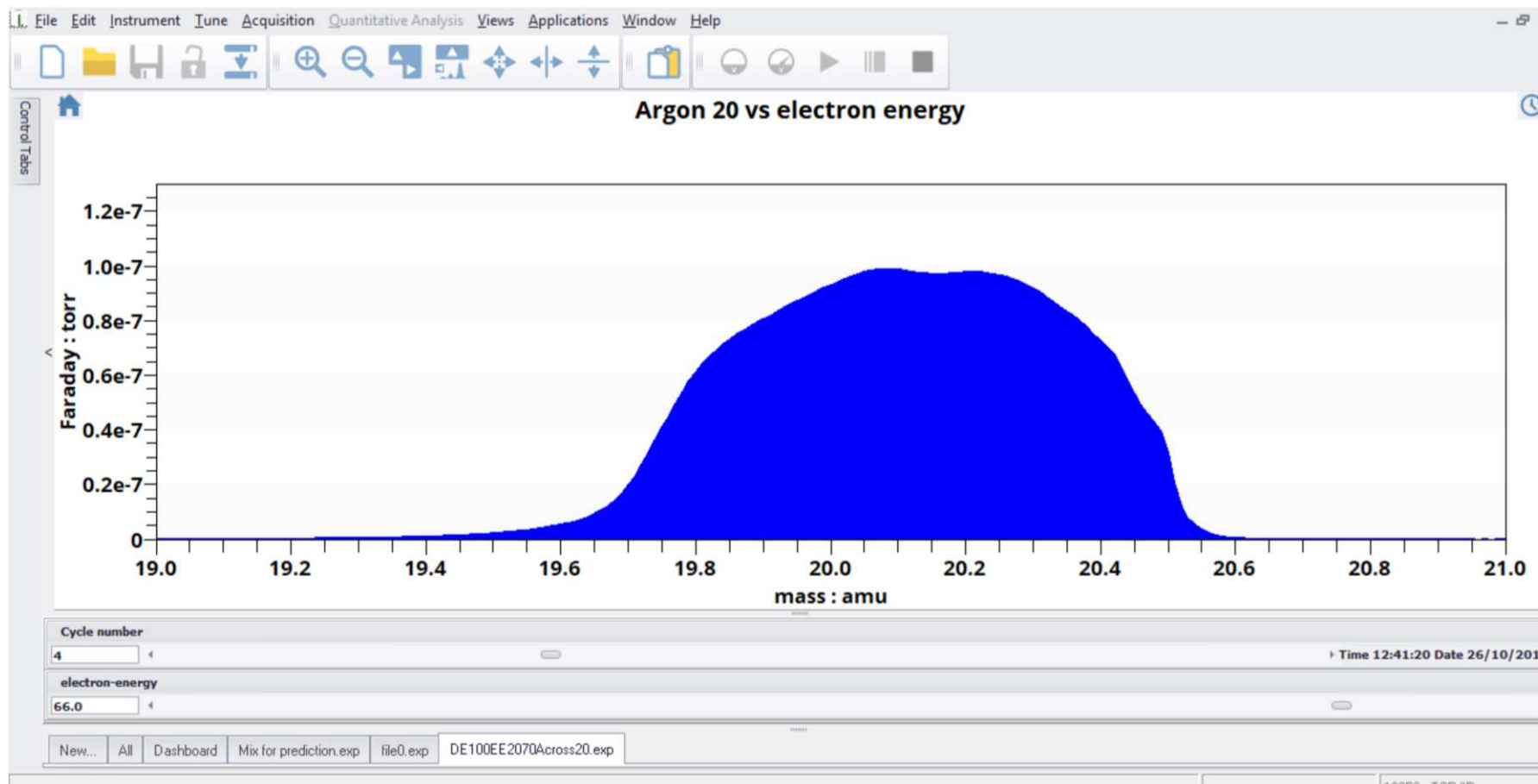


The new 3D data view allows users to view multi-variant scans in 3D.

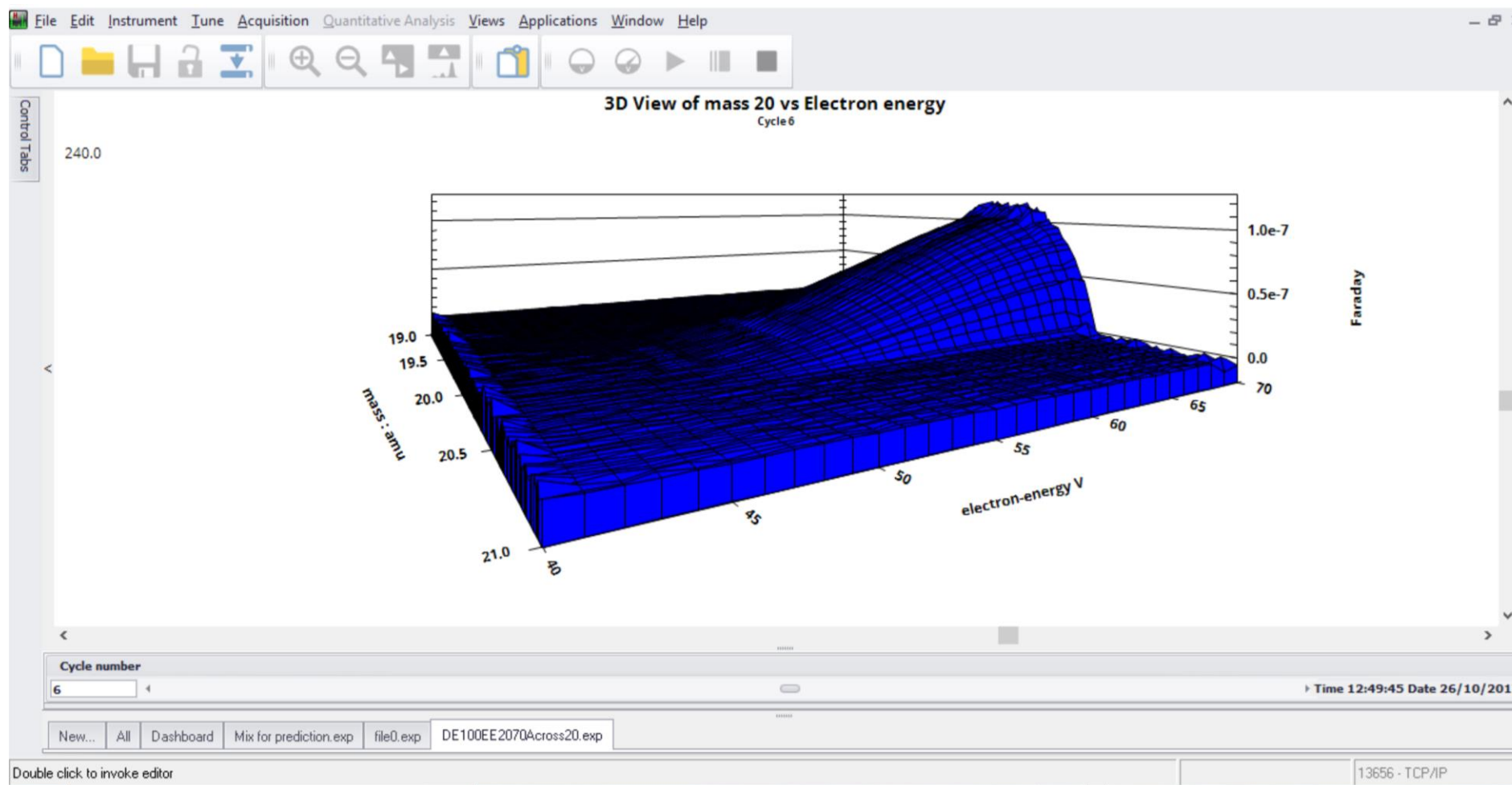
Multi-variant parameters include: mass, electron energy, focus and other ion optical lenses.

3D data - Argon mass 20 vs electron energy

APSI –MS appearance potential soft ionisation mass spectrometry

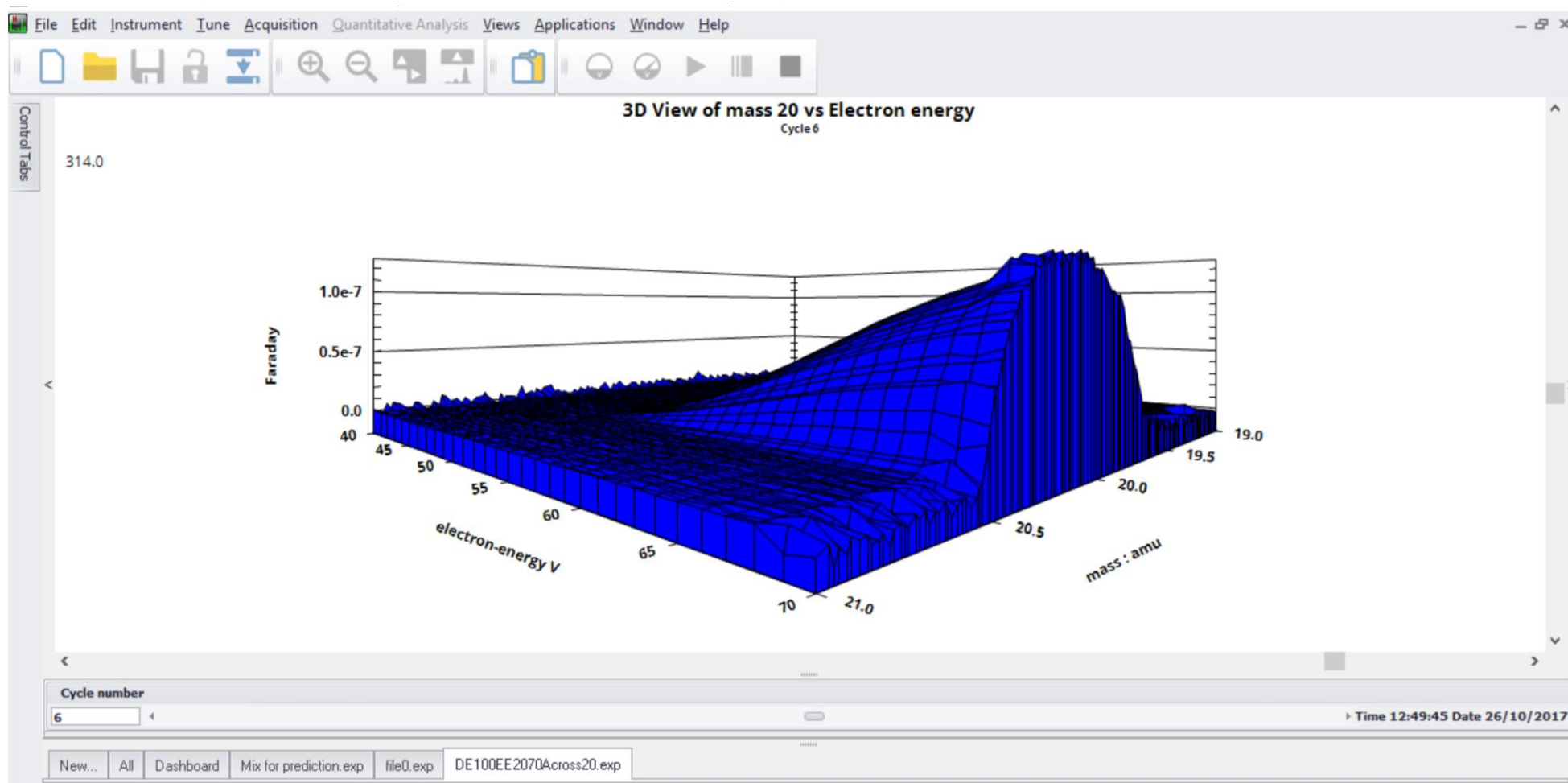


3D View of Argon mass 20 vs electron energy



APSI-MS:
Appearance
Potential Soft
Ionisation
Mass
Spectrometry

3D View of Argon mass 20 vs electron energy - rotated



APSI-MS:
Appearance
Potential Soft
Ionisation
Mass
Spectrometry