www.hidenanalytical.com
info@hiden.co.uk

HIDEN ANALYTICAL

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

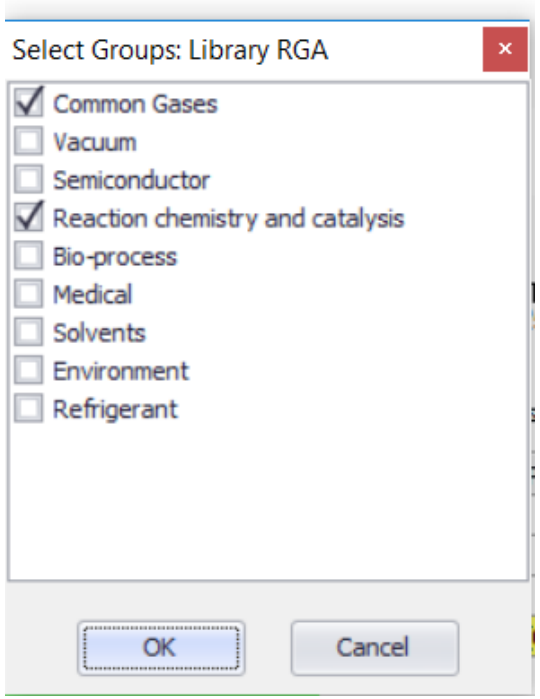
Tools for analysis include:

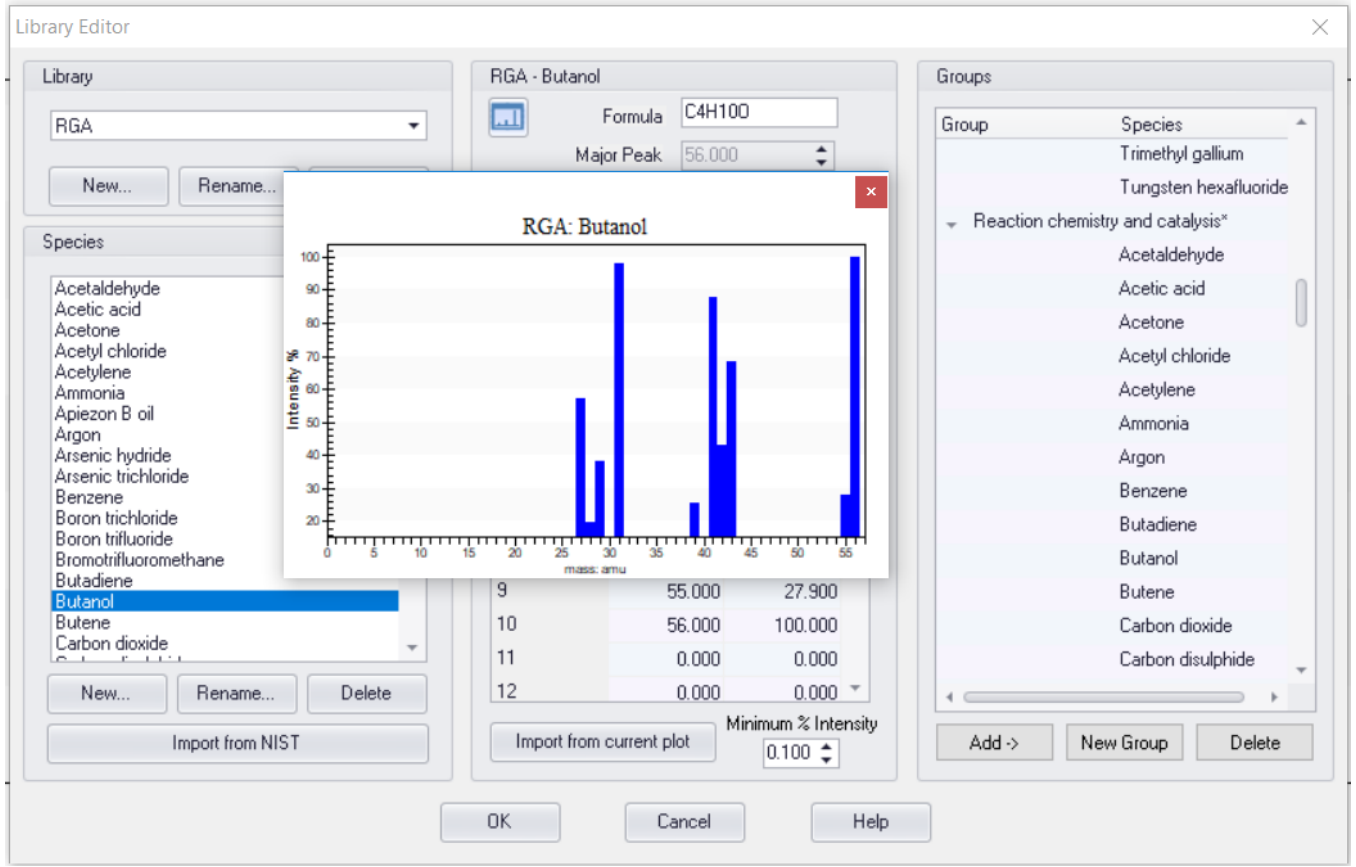
- Library groups edited and selected to be appropriate for the application.
- Peak identification – colour coded to indicate library match.
- Spectral simulation and subtraction tools providing difference spectra for comparison to recorded data.
- Parameter control to set thresholds for peak inclusion.

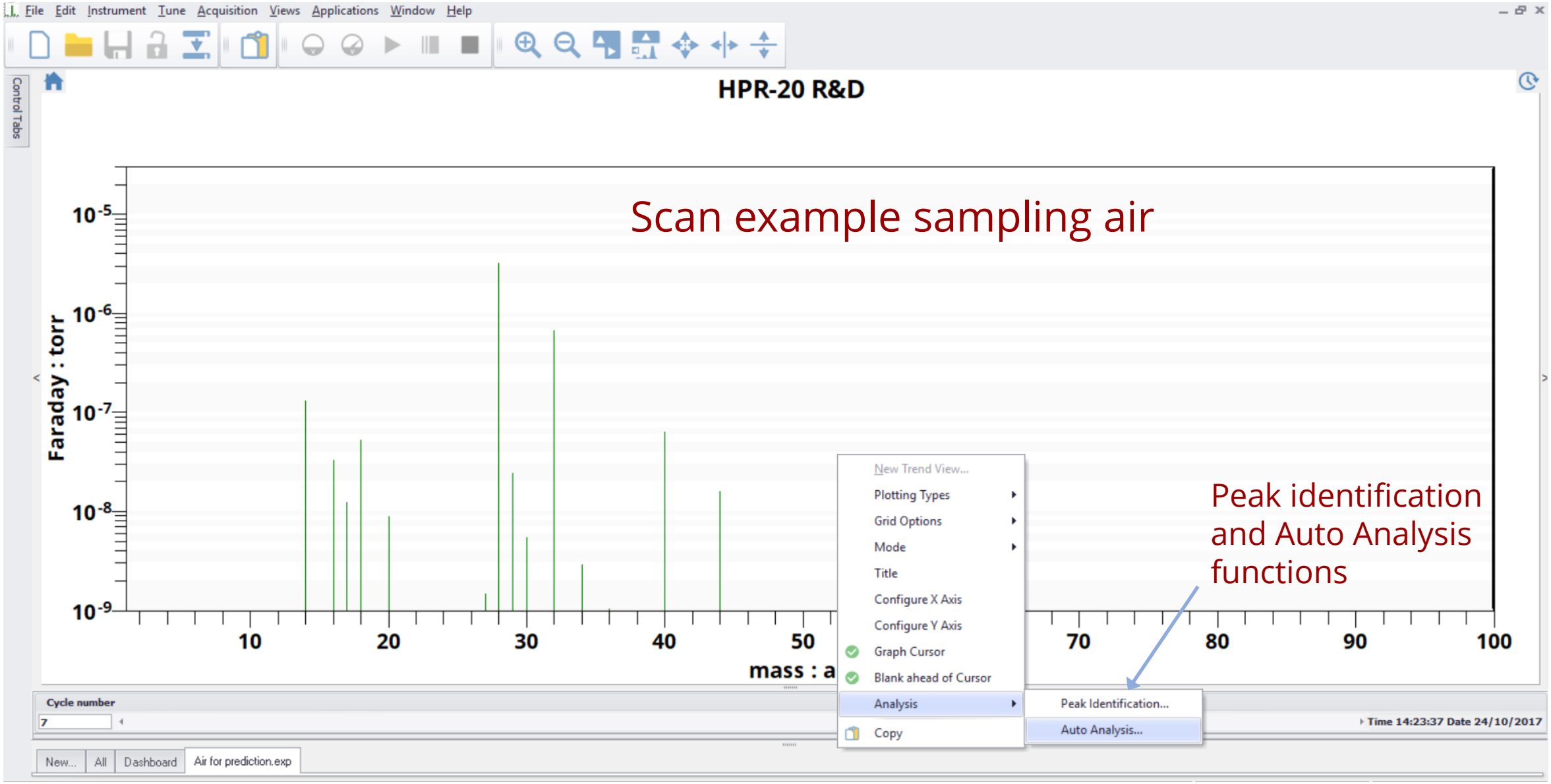
Library groups – enables application specific peak identification

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

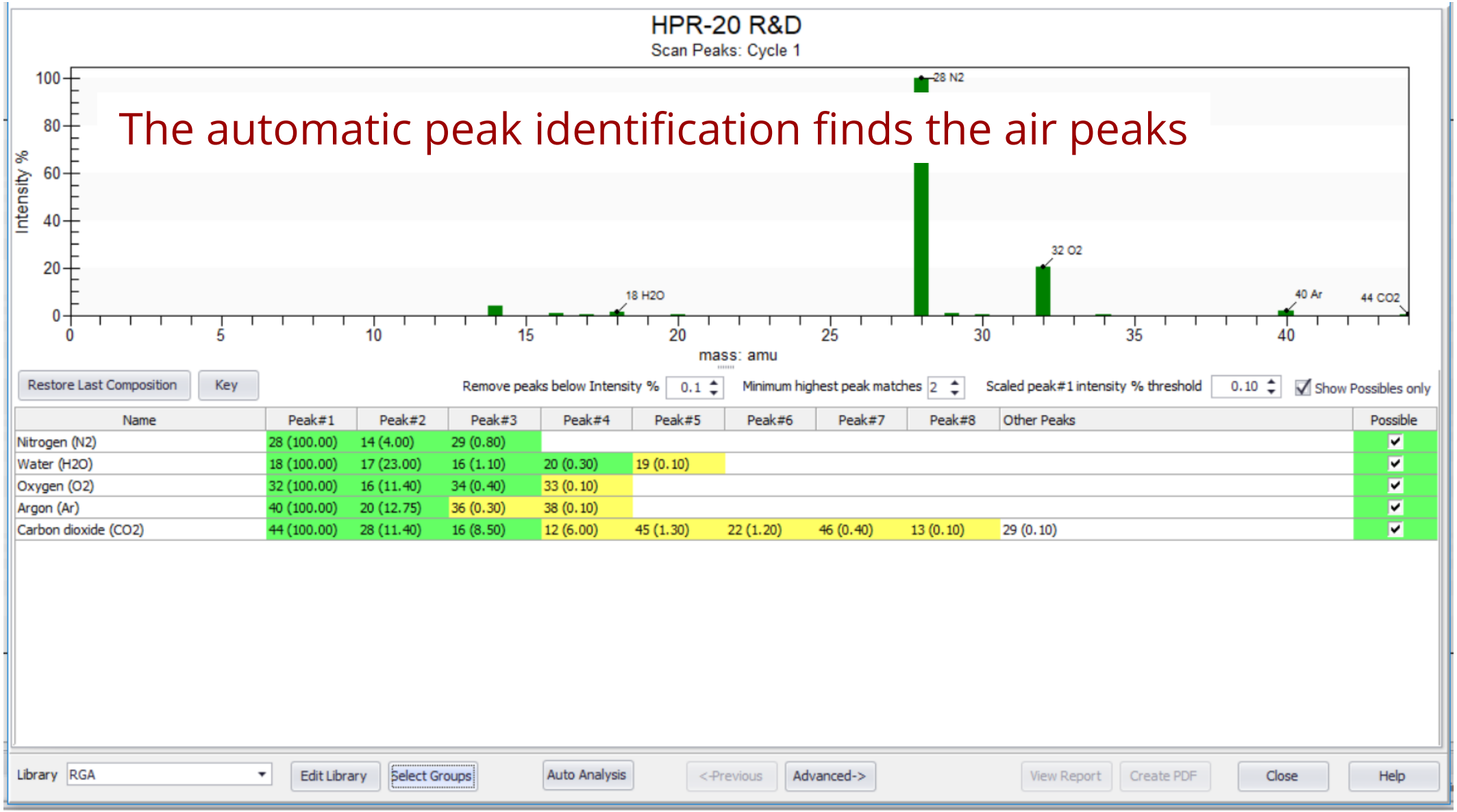
Default library groups include:






File Edit Instrument Tune Acquisition Views Applications Window Help
Control Tabs
HPR-20 R&D
Scan example sampling air
Faraday : torr
10-5
10-6
10-7
10-8
10-9
10 20 30 40 50 70 80 90 100
mass : a
New Trend View...
Plotting Types
Grid Options
Mode
Title
Configure X Axis
Configure Y Axis
Graph Cursor
Blank ahead of Cursor
Analysis
Copy
Peak Identification...
Auto Analysis...
Peak identification and Auto Analysis functions
Cycle number
7
Time 14:23:37 Date 24/10/2017
New... All Dashboard Air for prediction.exp

The automatic peak identification finds the air peaks



Name	Peak#1	Peak#2	Peak#3	Peak#4	Peak#5	Peak#6	Peak#7	Peak#8	Other Peaks	Possible
Nitrogen (N2)	28 (100.00)	14 (4.00)	29 (0.80)							✓
Water (H2O)	18 (100.00)	17 (23.00)	16 (1.10)	20 (0.30)	19 (0.10)					✓
Oxygen (O2)	32 (100.00)	16 (11.40)	34 (0.40)	33 (0.10)						✓
Argon (Ar)	40 (100.00)	20 (12.75)	36 (0.30)	38 (0.10)						✓
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)	✓

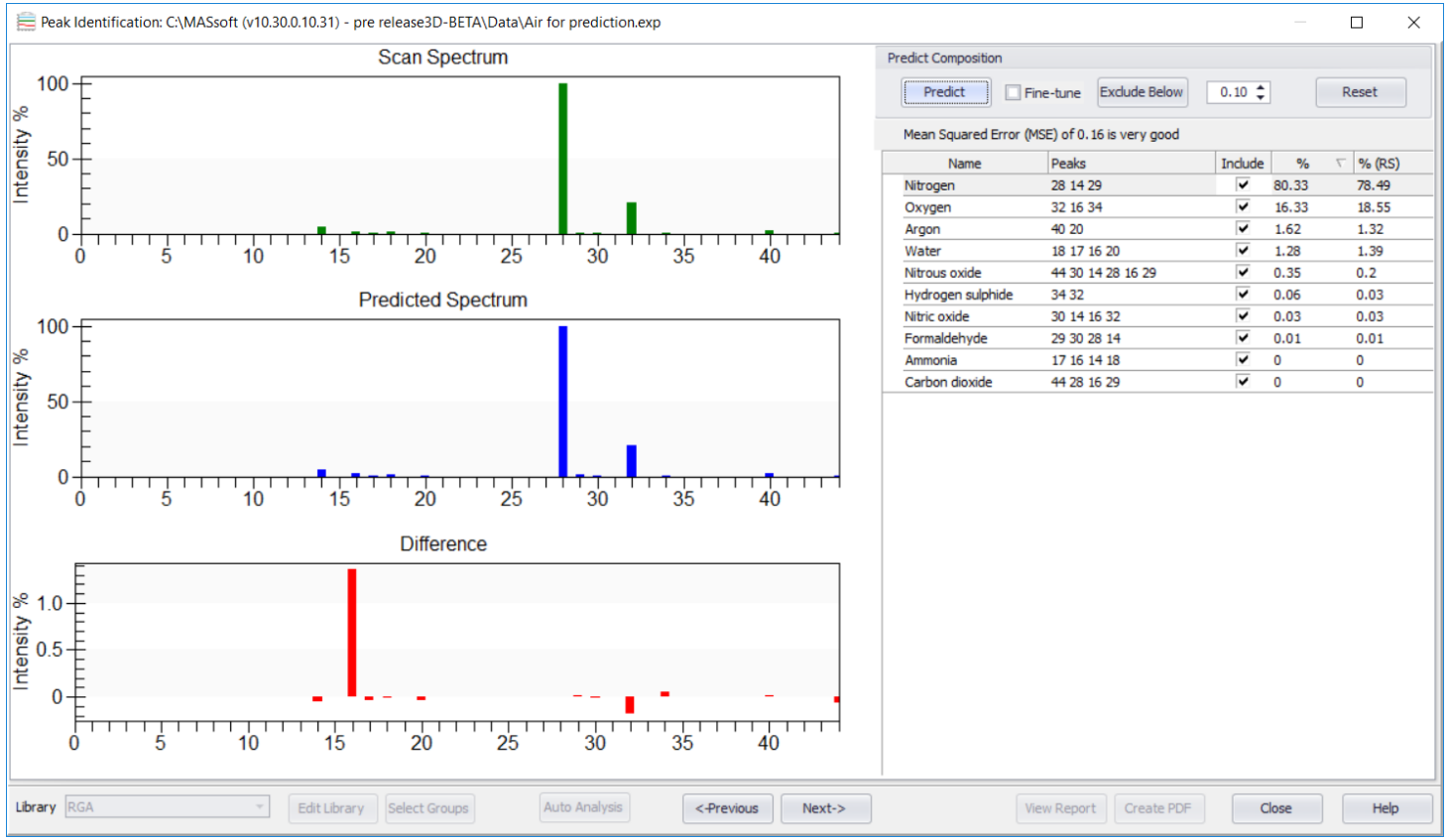
Recorded, predicted and difference spectra

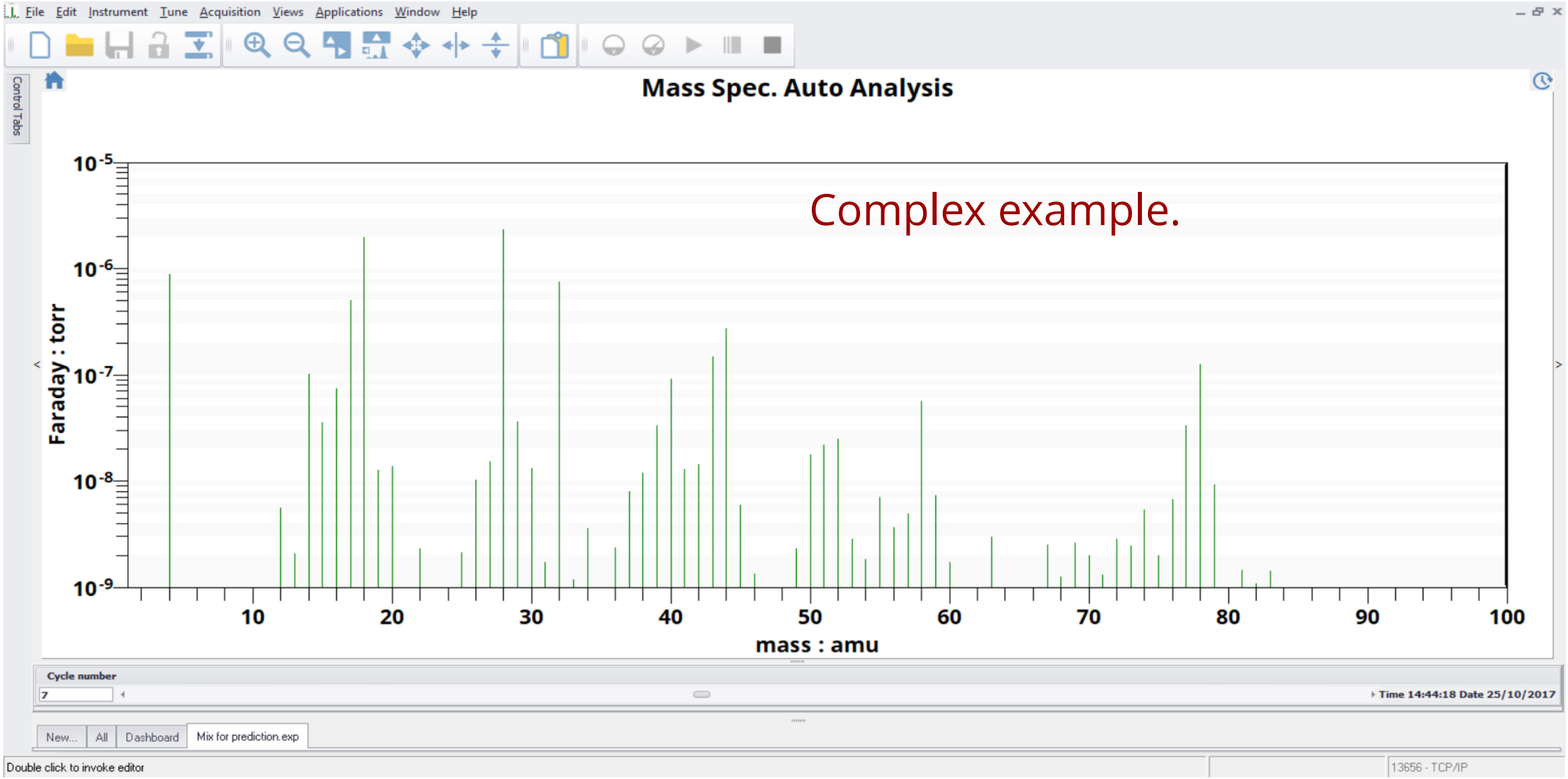
Peak identification and automatic analysis:

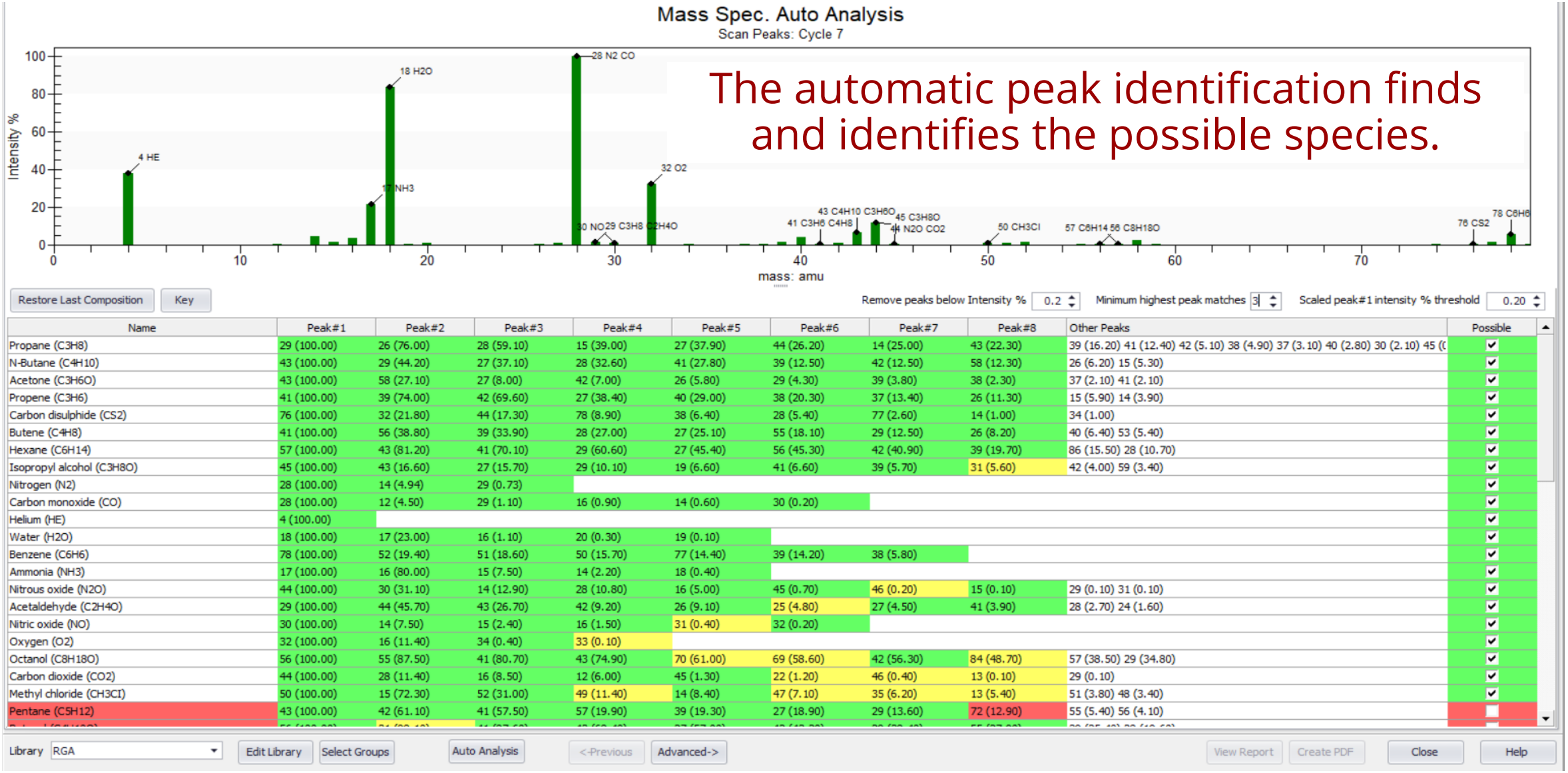
MASsoft includes predictive genetic algorithms to evaluate spectra, identify species present and calculate the gas composition.

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.




File Edit Instrument Tune Acquisition Views Applications Window Help
Control Tabs
Mass Spec. Auto Analysis
Complex example.
Faraday : torr
10-5
10-6
10-7
10-8
10-9
10 20 30 40 50 60 70 80 90 100
mass : amu
Cycle number
7
Time 14:44:18 Date 25/10/2017
New... All Dashboard Mix for prediction.exp
Double click to invoke editor
13656 - TCP/IP



The automatic peak identification finds and identifies the possible species.

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 (	✓
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)	

Analysis Report - PDF

The report includes:

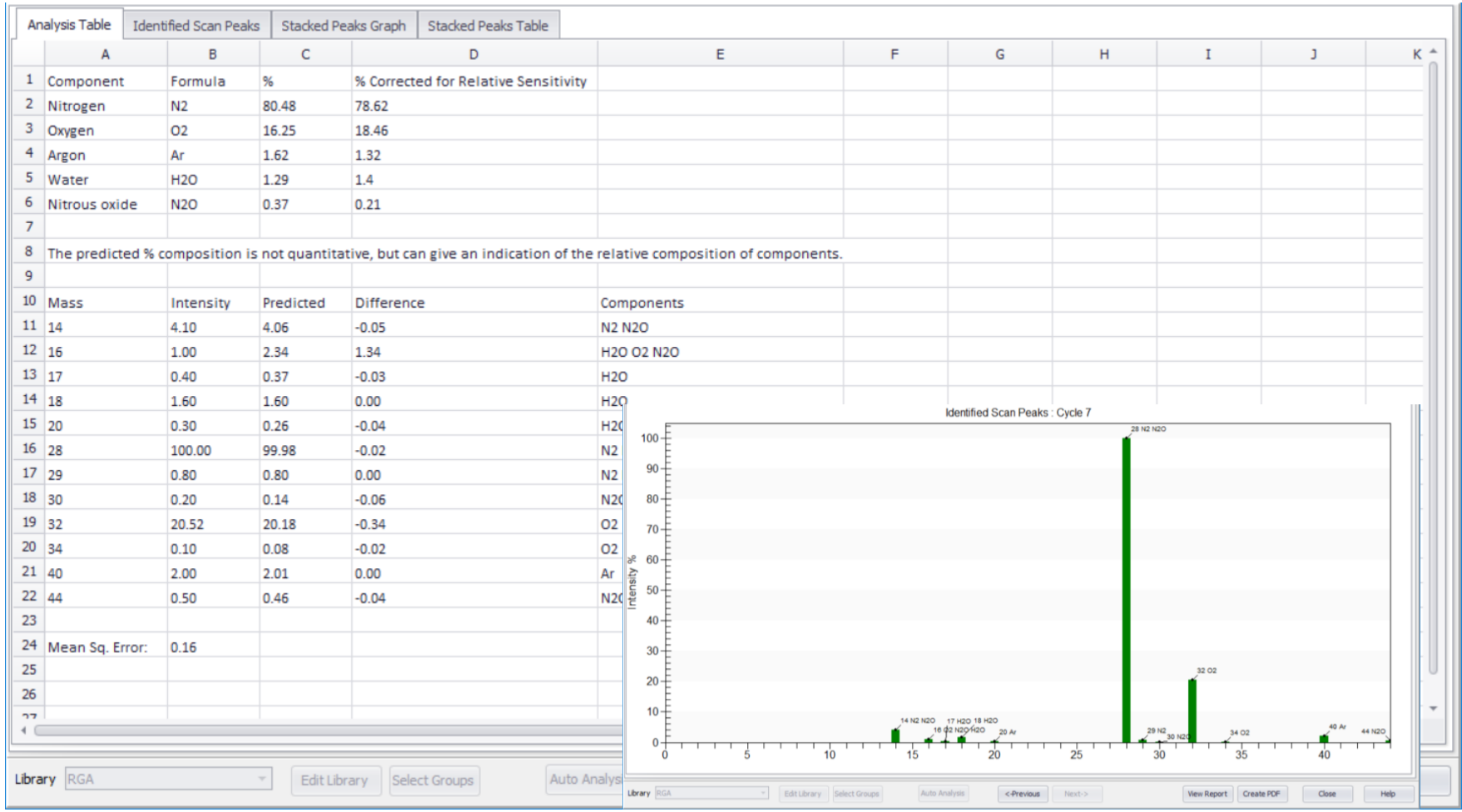
Species with % composition.

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.

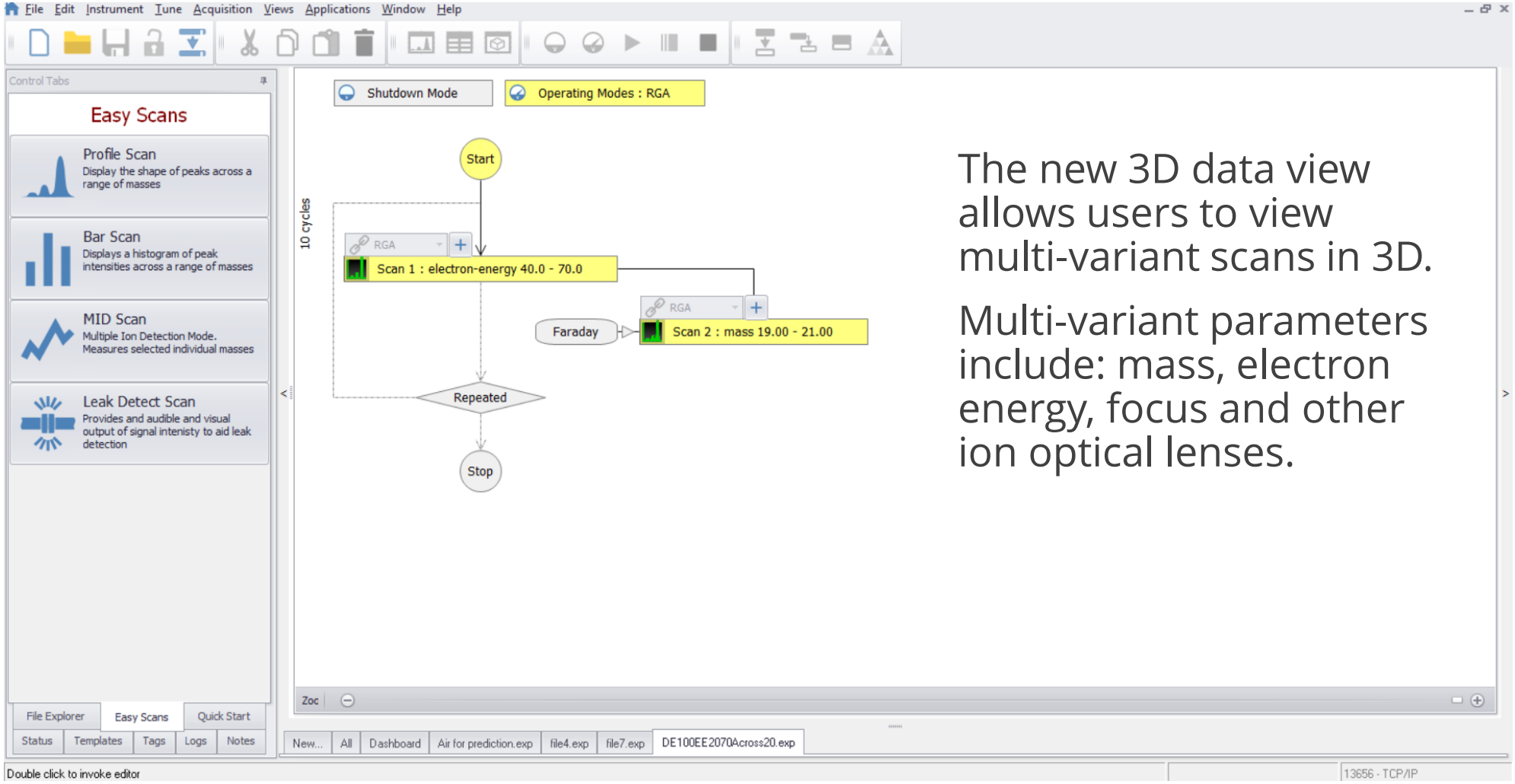
The analysis report is exported as a PDF.



Analysis Table | Identified Scan Peaks | Stacked Peaks Graph | Stacked Peaks Table

	A	B	C	D	E
1	Component	Formula	%	% Corrected for Relative Sensitivity	
2	Nitrogen	N2	80.48	78.62	
3	Oxygen	O2	16.25	18.46	
4	Argon	Ar	1.62	1.32	
5	Water	H2O	1.29	1.4	
6	Nitrous oxide	N2O	0.37	0.21	
7					
8	The predicted % composition is not quantitative, but can give an indication of the relative composition of components.				
9					
10	Mass	Intensity	Predicted	Difference	Components
11	14	4.10	4.06	-0.05	N2 N2O
12	16	1.00	2.34	1.34	H2O O2 N2O
13	17	0.40	0.37	-0.03	H2O
14	18	1.60	1.60	0.00	H2O
15	20	0.30	0.26	-0.04	H2O
16	28	100.00	99.98	-0.02	N2
17	29	0.80	0.80	0.00	N2
18	30	0.20	0.14	-0.06	N2O
19	32	20.52	20.18	-0.34	O2
20	34	0.10	0.08	-0.02	O2
21	40	2.00	2.01	0.00	Ar
22	44	0.50	0.46	-0.04	N2O
23					
24	Mean Sq. Error:	0.16			
25					
26					

3D Data View

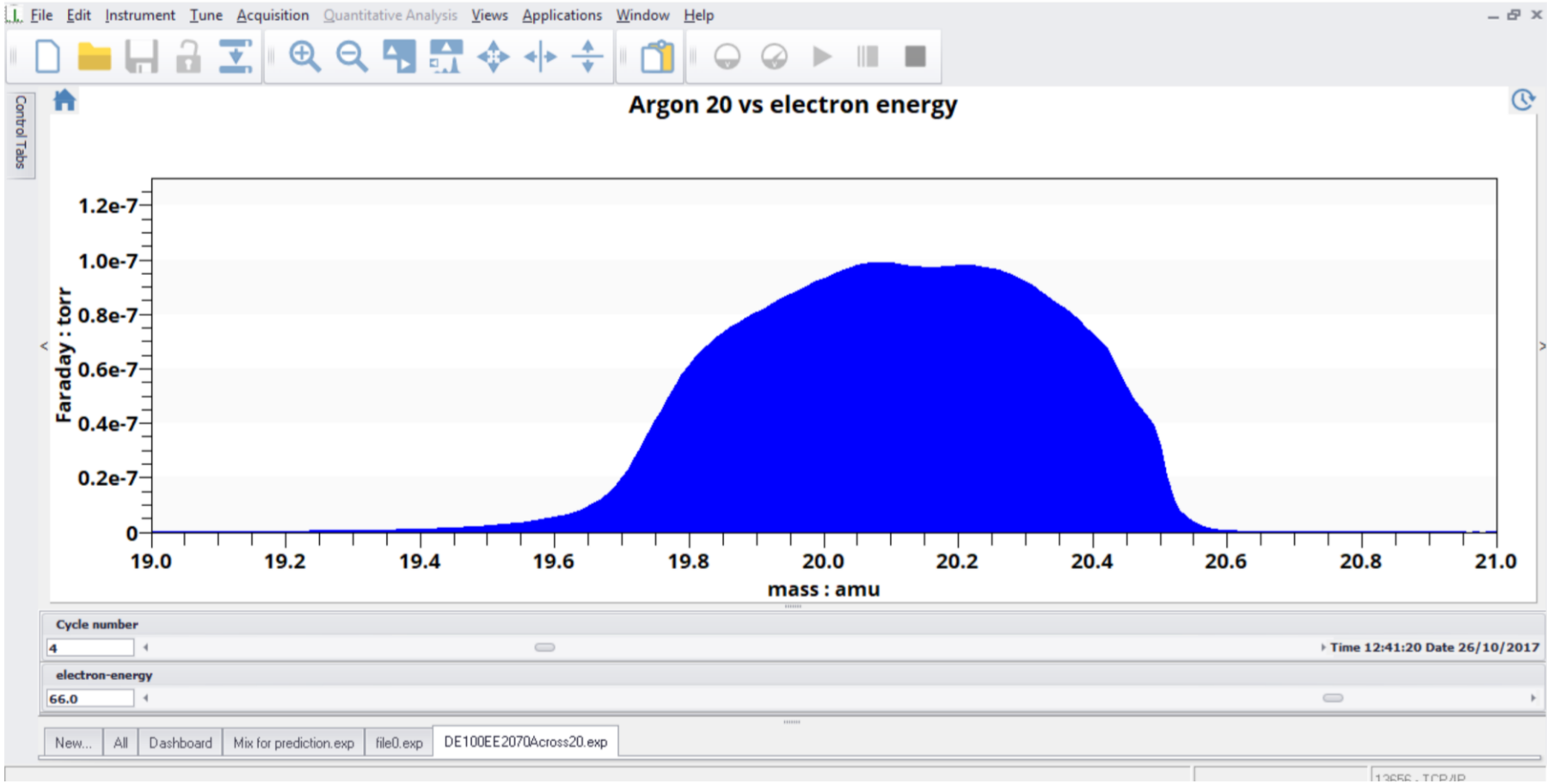


The new 3D data view allows users to view multi-variant scans in 3D.

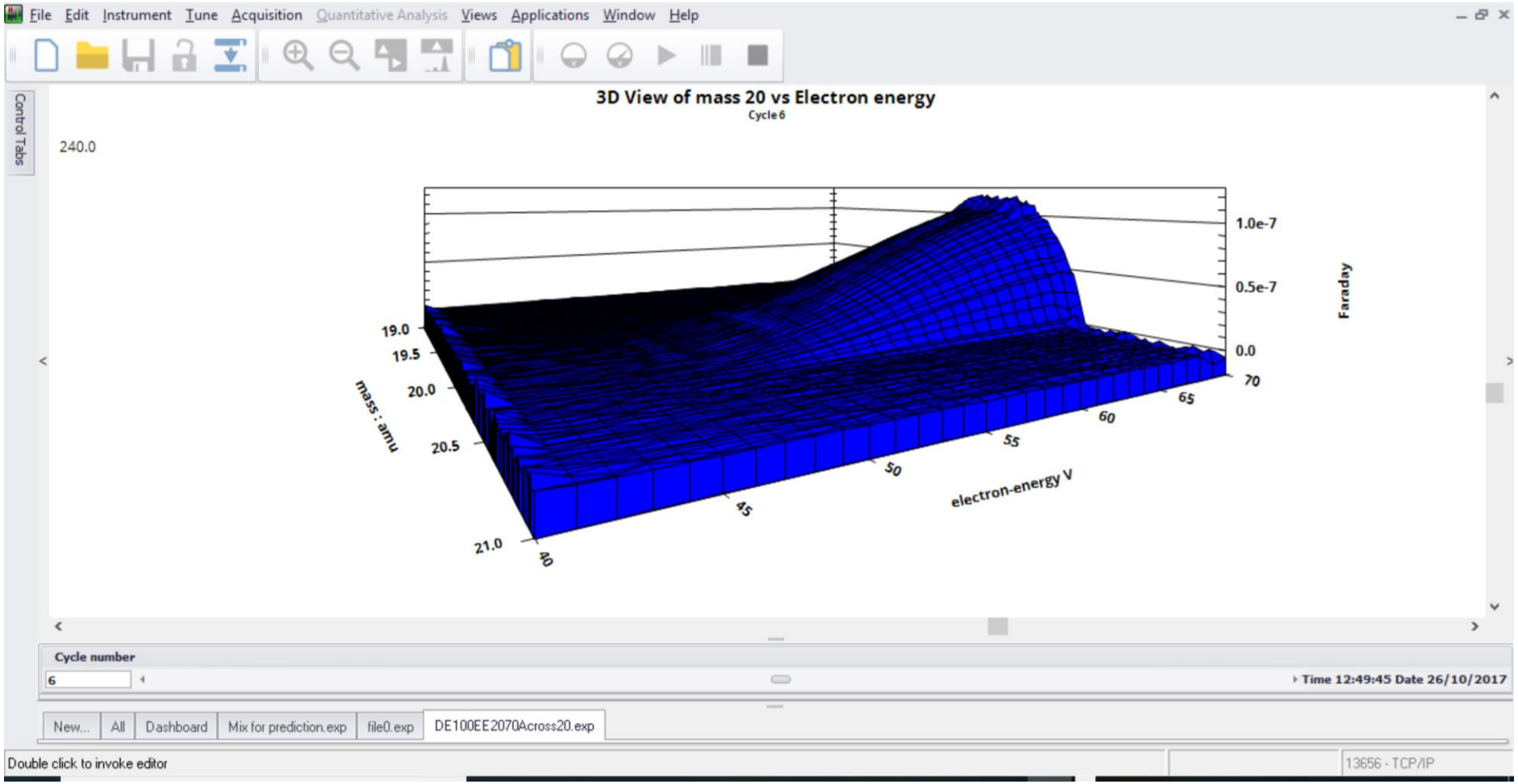
Multi-variant parameters include: mass, electron energy, focus and other ion optical lenses.

3D data - Argon mass 20 vs electron energy

APSI –MS appearance potential soft ionisation mass spectrometry

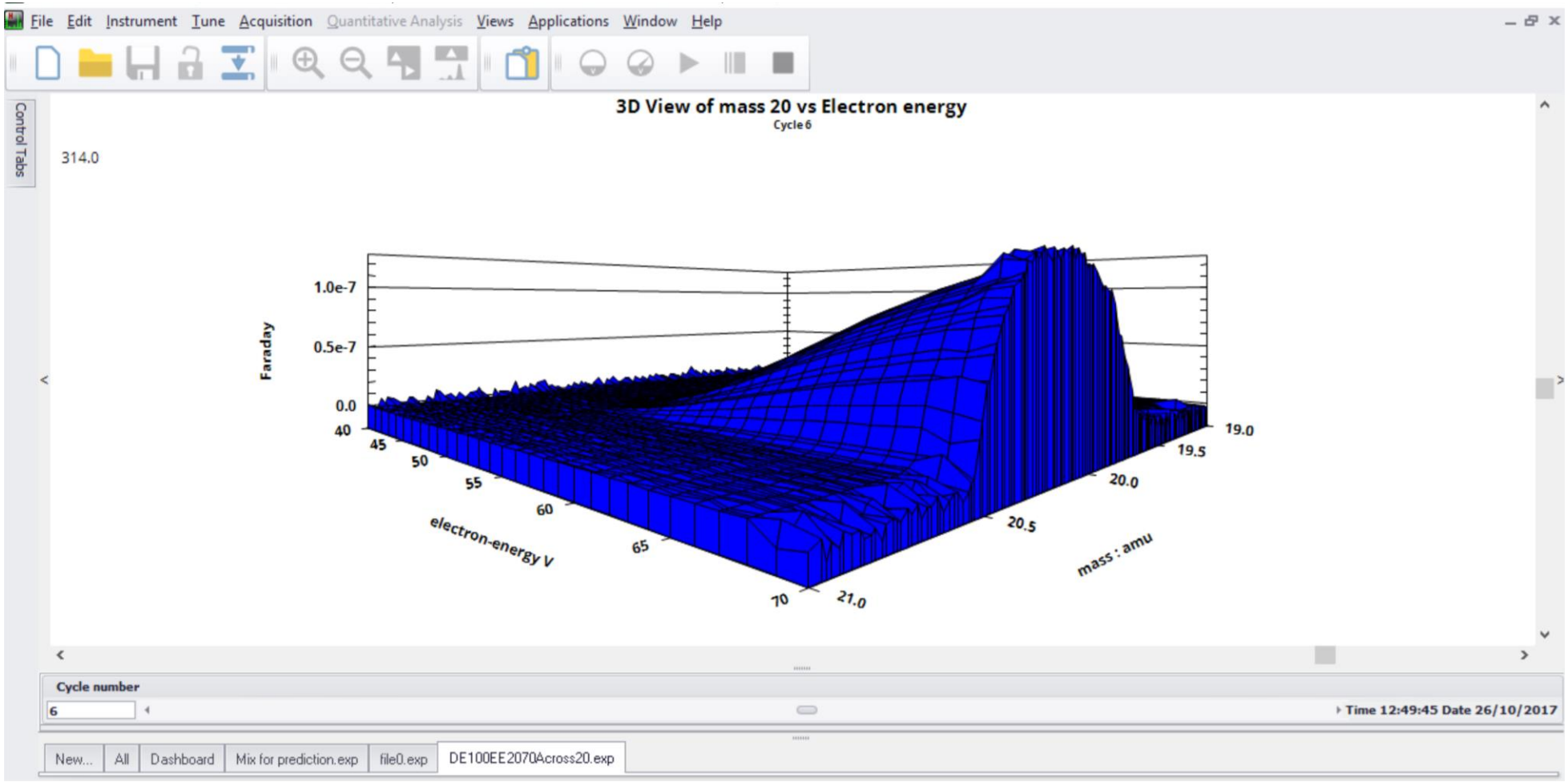


3D View of Argon mass 20 vs electron energy



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