

Hidden QGA 2

Quantitative Gas Analysis Software

Introduction

Hidden QGA 2 quantitative gas analysis software is for quantitative analysis of **gases and vapours**, and is offered with Hidden's gas analysis systems.

QGA software is designed for use by users with or without experience of mass spectrometry.

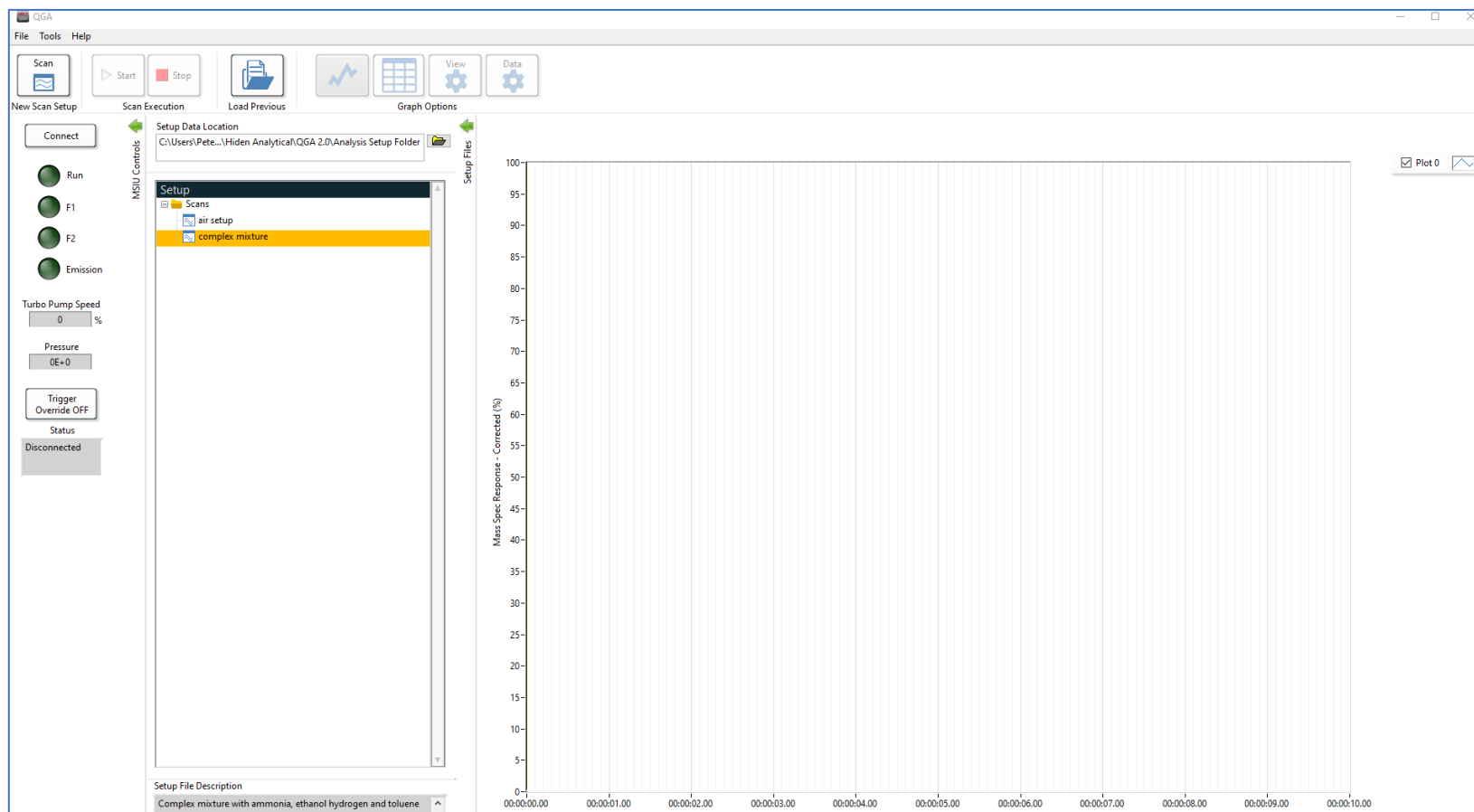
Set-up screens are intuitive and easy to navigate.

A calibration wizard guides the user through an automated procedure.

Raw data, corrected data and quantitative data is acquired, displayed (graphical and tabular formats) and saved in real time.

Data export on the fly to MS Excel and to tags for OPC compatible clients is included.

QGA 2 - Home Screen



Three control sections for instrument comms, analysis, data view/export.
Two display areas with mass spectral evaluator, emulating the iPad app.

QGA 2 – Gas Analysis Recipe Set-Up

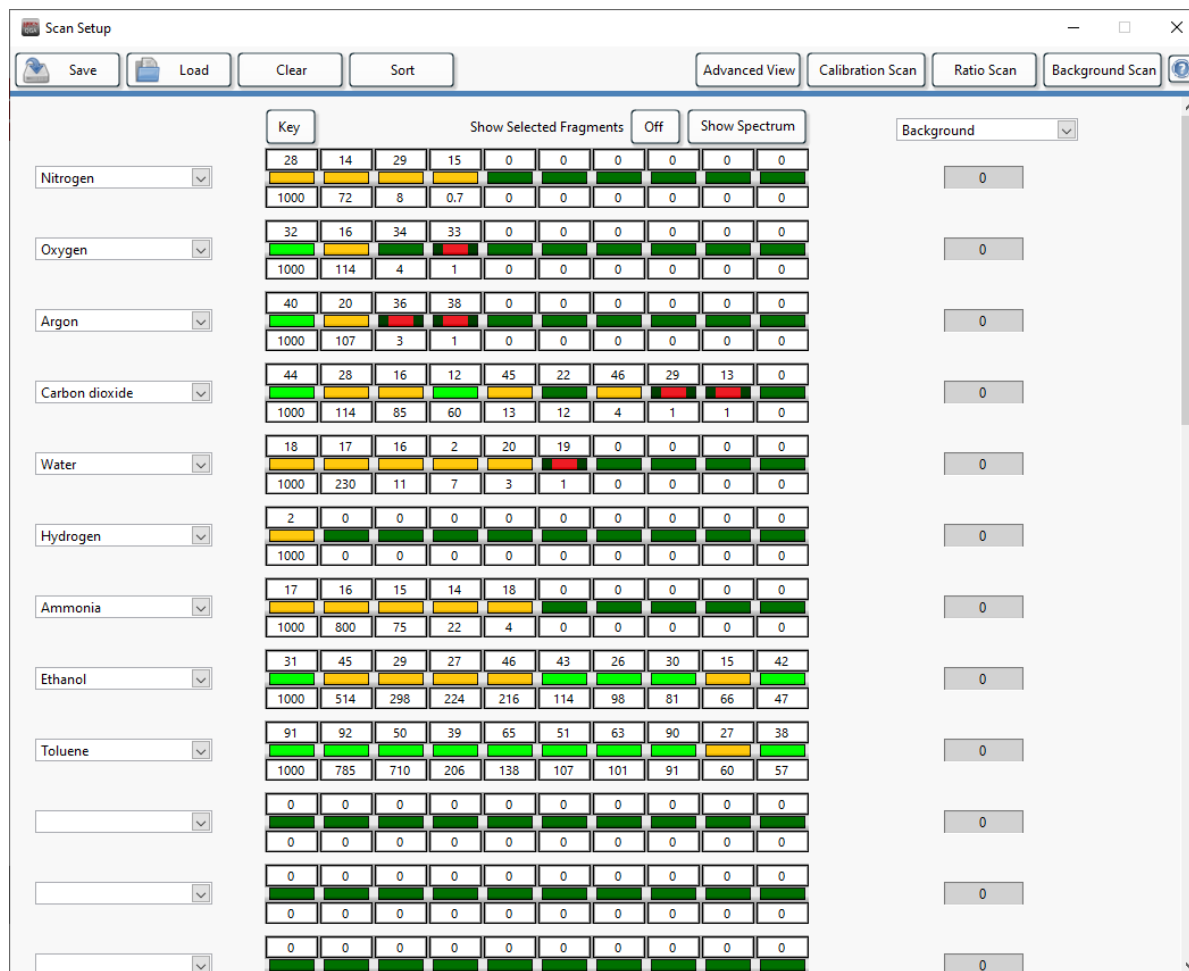
Gas and vapours included for analysis are selected from the library. The MS evaluator automatically selects the optimum mass peaks to complete the analysis. Recipes can be edited, saved and exported.

The screenshot shows the 'Scan Setup' window with a table of mass peaks for various gases. The table has columns for 'Key' and 'Show Selected Fragments' (On) and 'Show Spectrum'. The gases listed are Nitrogen, Oxygen, Argon, Carbon dioxide, Water, Hydrogen, Ammonia, Ethanol, and Toluene. The table shows the mass-to-charge ratio (m/z) and relative intensity for each peak.

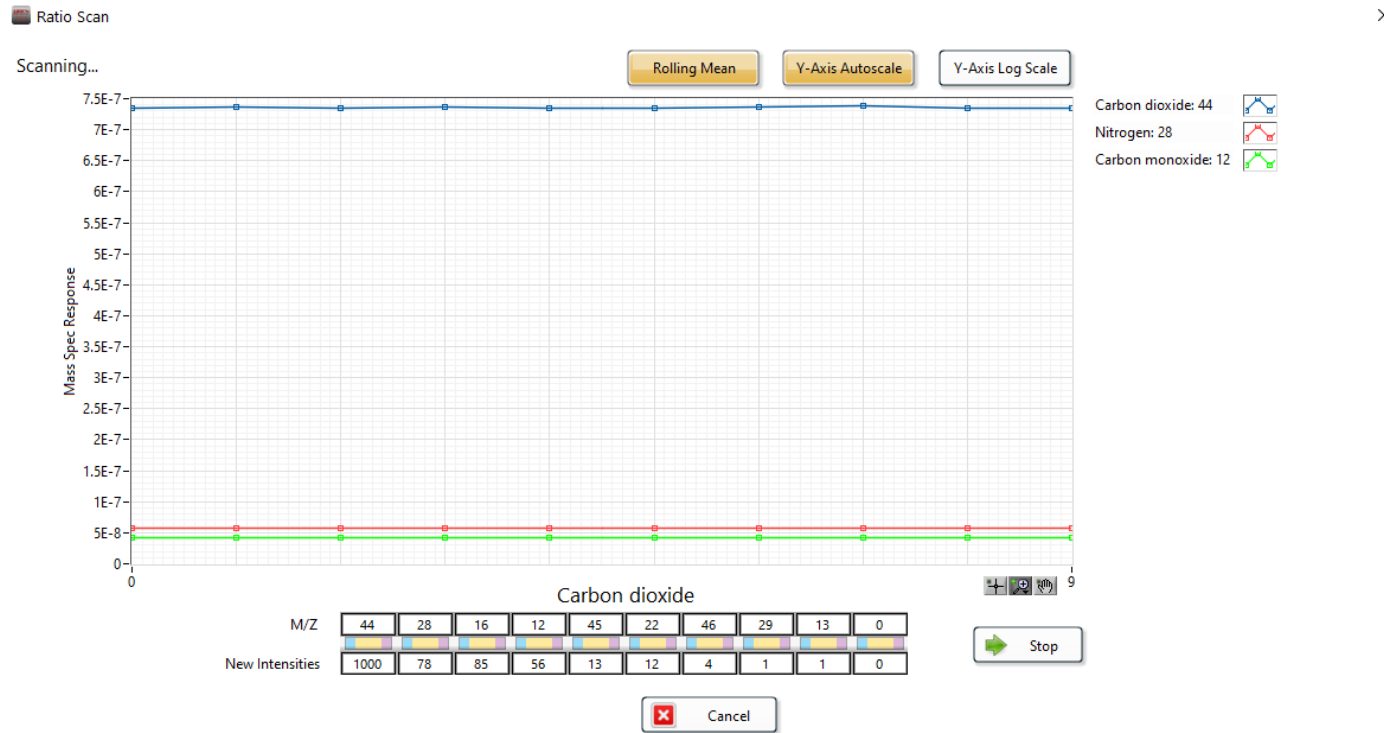
Gas	Key	28	14	29	15	0	0	0	0	0
Nitrogen	1000	72	8	0.7	0	0	0	0	0	0
Oxygen	32	16	34	33	0	0	0	0	0	0
Oxygen	1000	114	4	1	0	0	0	0	0	0
Argon	40	20	36	38	0	0	0	0	0	0
Argon	1000	107	3	1	0	0	0	0	0	0
Carbon dioxide	44	28	16	12	45	22	46	29	13	0
Carbon dioxide	1000	114	85	60	13	12	4	1	1	0
Water	18	17	16	2	20	19	0	0	0	0
Water	1000	230	11	7	3	1	0	0	0	0
Hydrogen	2	0	0	0	0	0	0	0	0	0
Hydrogen	1000	0	0	0	0	0	0	0	0	0
Ammonia	17	16	15	14	18	0	0	0	0	0
Ammonia	1000	800	75	22	4	0	0	0	0	0
Ethanol	31	45	29	27	46	43	26	30	15	42
Ethanol	1000	514	298	224	216	114	98	81	66	47
Toluene	91	92	50	39	65	51	63	90	27	38
Toluene	1000	785	710	206	138	107	101	91	60	57
	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0
	0	0	0	0	0	0	0	0	0	0

QGA 2 – Gas Analysis Recipe Set-Up

The gas set up can be viewed with filter 'off' as above or 'on' as shown in the previous slide. The filter off setting combined with the peak limit settings allows an advanced user to optimise peak selection for analysis.

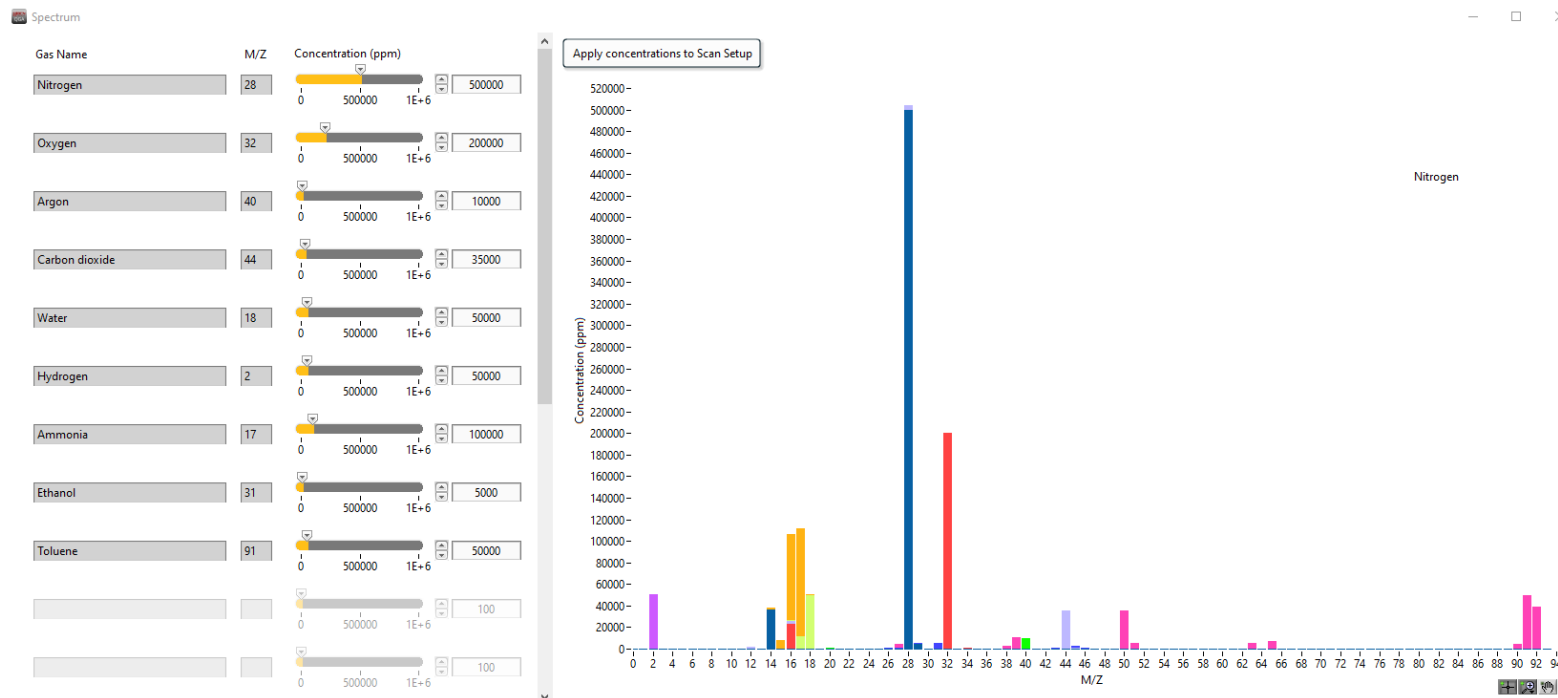


QGA - Ratio Analysis



The ratio analysis wizard ensures the fragment ratios used in any calculations are applicable to the specific setup and so improves accuracy.

QGA 2 – Spectrum Analysis



The Spectrum analysis tool allows the user to view the effect of different concentrations on the overall spectrum. By applying the expected concentrations to the scan setup, settings are automatically adjusted to ensure the most applicable fragment mass is selected for each gas.

QGA 2 - Advanced settings

Advanced settings provide for control of the dynamic range, the soft ionisation parameters (emission current and electron energy), detector and the scan speed for each gas.

	Autorange High	Start Range	Autorange Low	Settle Time	Dwell Time	Electron Energy	Emission Current	Detector
Nitrogen	-5	-5	-10	Normal	Normal	70	400	Faraday
Oxygen	-5	-5	-10	Normal	Normal	70	400	Faraday
Argon	-5	-5	-10	Normal	Normal	70	400	Faraday
Carbon dioxide	-7	-7	-13	Normal	Normal	70	400	SEM
Water	-7	-7	-13	Normal	Normal	70	400	SEM
Hydrogen	-7	-7	-13	Normal	Normal	70	500	SEM
Ammonia	-7	-7	-13	Normal	Normal	70	500	SEM
Ethanol	-7	-7	-13	Normal	Normal	70	500	SEM
Toluene	-7	-7	-13	Normal	Normal	70	500	SEM
	-7	-7	-13	Normal	Normal	70	400	SEM
	-7	-7	-13	Normal	Normal	70	400	SEM
	-7	-7	-13	Normal	Normal	70	400	SEM

QGA 2 - Calibration Wizard

Calibration Scan Wizard



Multi Cylinder/ Multi Point Scan Values

Test	Nitrogen Measured	Nitrogen Actual	Nitrogen RS	Oxygen Measured	Oxygen Actual	Oxygen RS	Argon Measured	Argon Actual	Argon RS	Carbon dioxide Measured	Carbon dioxide Actual	Carbon dioxide RS
1	805758	781000	1.00	188646	209000	0.875	5445.74	9600.00	0.550	149.513	400.000	0.362
2	807598	800000	1.00	186938	190000	0.975	5351.41	9000.00	0.589	112.739	1000.00	0.112
3	809370	810000	1.00	185537	184500	1.01	4948.21	5000.00	0.990	145.140	500.000	0.291

 %

Gas Name	Linear Regression	R (Linearity)
Nitrogen	$y = -0.000000x + 1.000000$	1.0000
Oxygen	$y = -0.428808x + 8.972417$	0.9467
Argon	$y = -9.182233x + 5.529002$	0.9902
Carbon dioxide	$y = 63.289948x - 0.604633$	0.9704

Values used to calculate the final RS are highlighted in the table. If a RS value is an outlier then reject by clicking on the value in the table.

+ Add to Setup

➔ Finish

The Calibration Wizard simplifies calibration and automatically calculates sensitivity factors. Options of single mix calibrations, multiple mix or multipoint calibration for improved accuracy.

QGA 2 - Background Subtraction Wizard

Background Scan Wizard

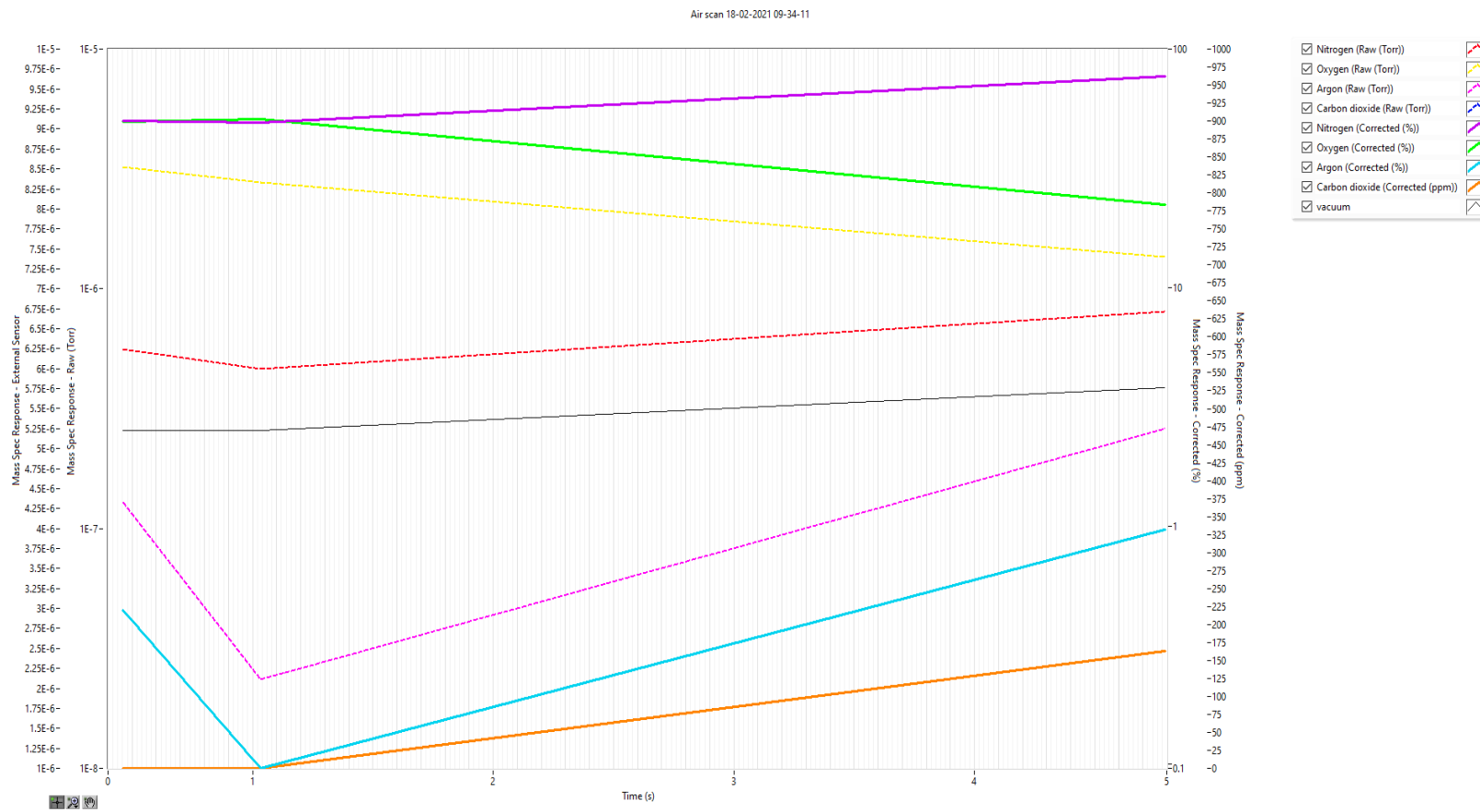
- □ ×

Review background

Gas Name	Background	M/Z Peak	Background Taken
Carbon dioxide	1.5151E-10	44	11:40:00 01/02/21

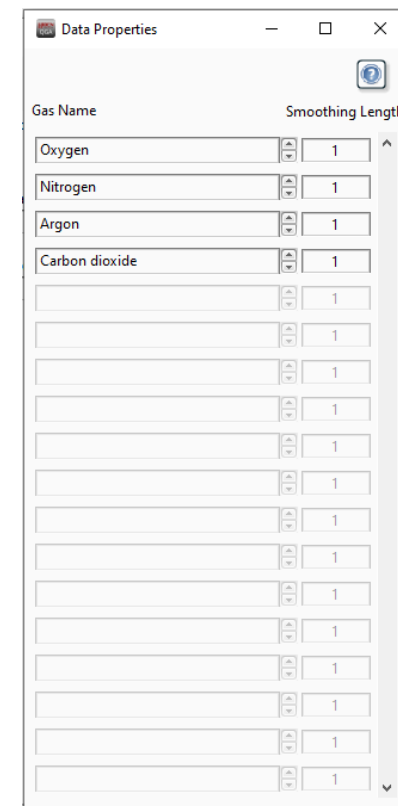
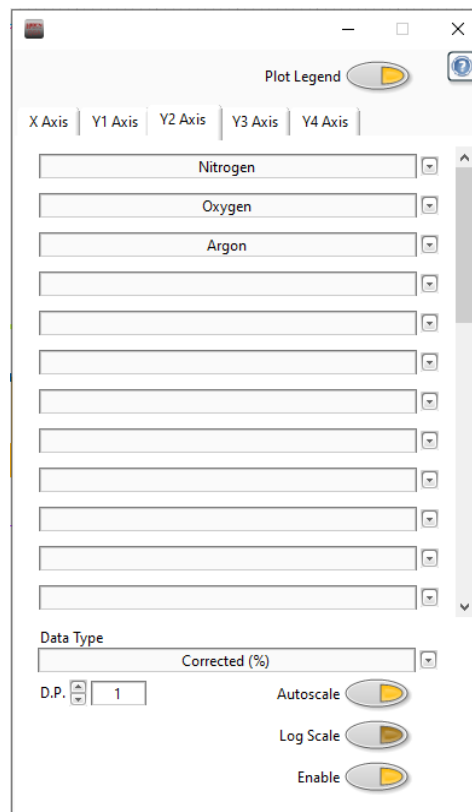
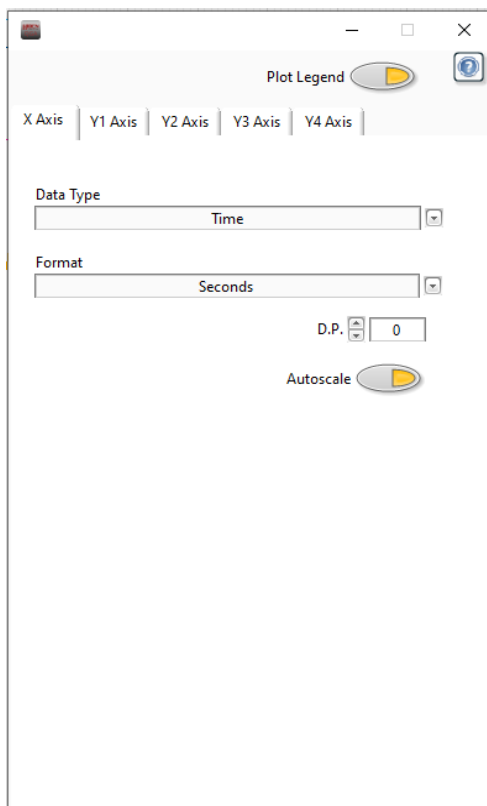
The instrument connected to a 'zero' gas can automatically scan the instrument 'background signal' for any selected gas. Measured data is automatically corrected for the background levels recorded. Applicable for measurements at PPM concentration levels for species including: CO₂, Water, Hydrogen, CO and Nitrogen

QGA 2 – Real Time Data Display



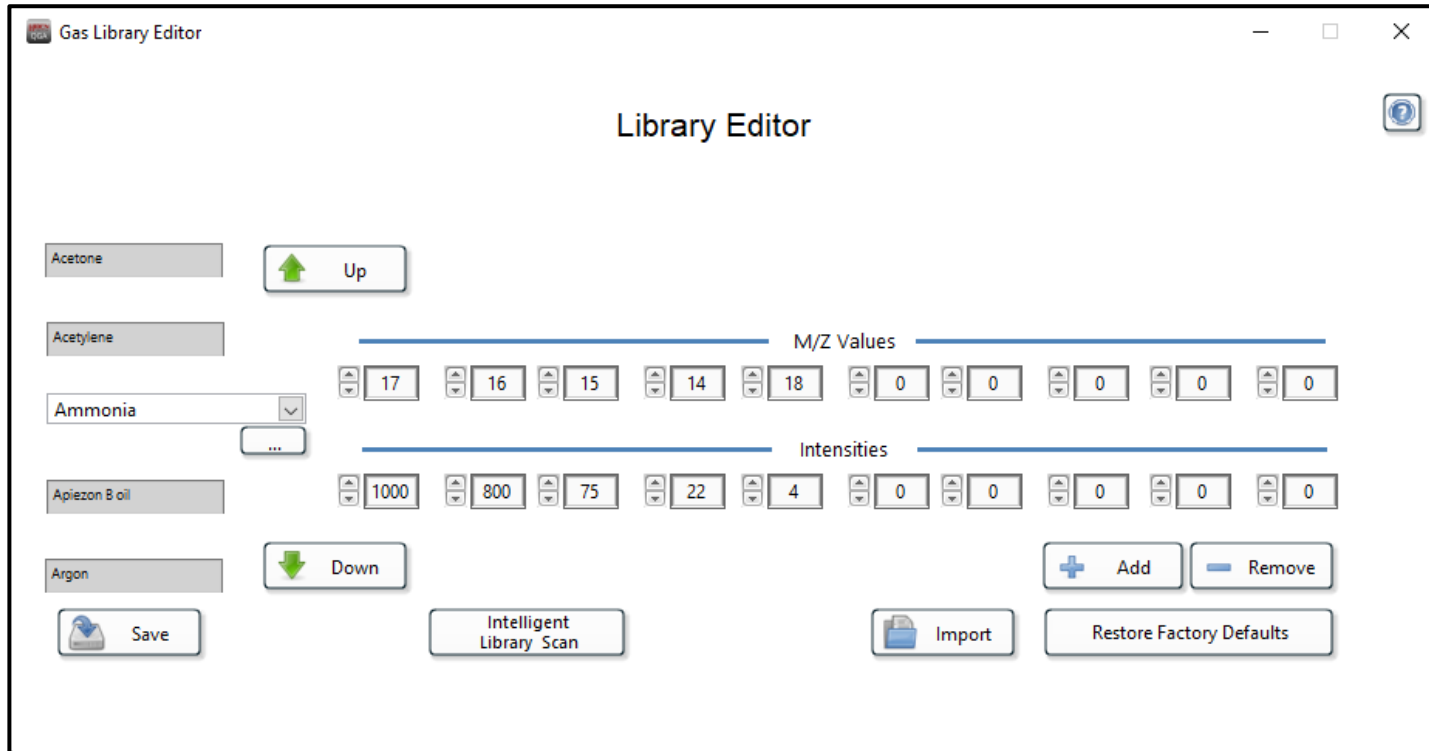
Graphical and tabular display with 4 y-axis control, displaying concentration, raw data, corrected data or external device data

QGA 2 – Real Time Data Display



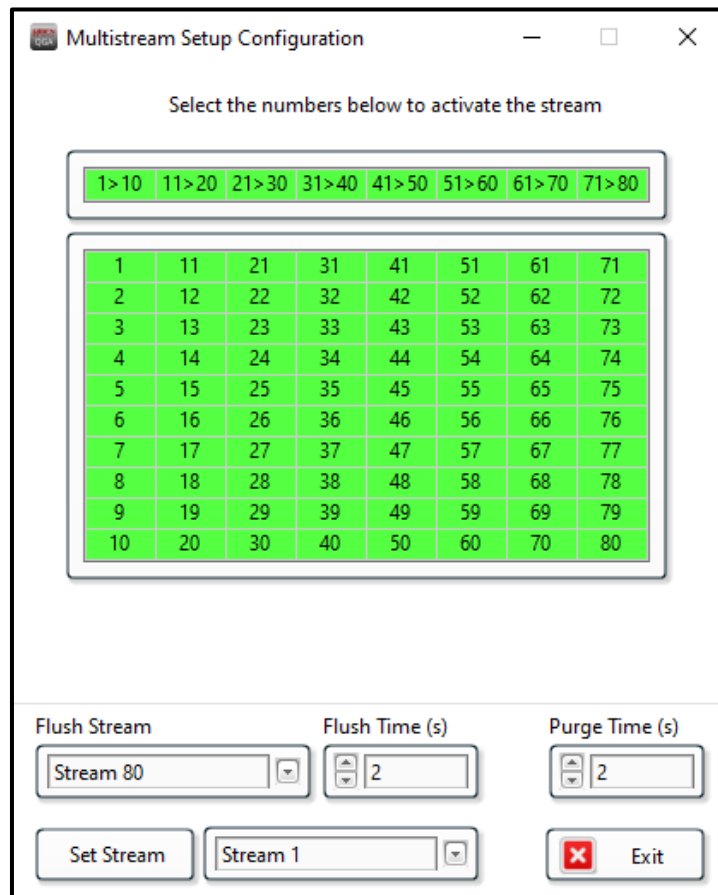
Display time or external device data on the X axis. Multiple options for Y axis. Data smoothing option

QGA 2 - Library Editor



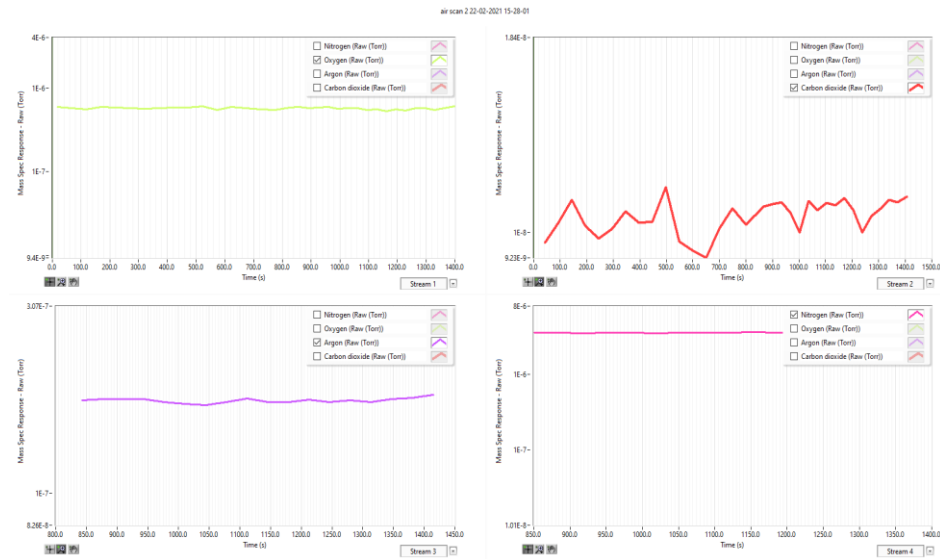
The library editor includes the 'Intelligent Library Scan' feature that automatically corrects the library entry for a given gas for specific instrument settings.

QGA 2 - Multistream



QGA multi-stream includes control for multi stream gas sampling inlets, with up to 80 streams. The sample stream sequence is fully editable before and during analysis.

QGA 2 - Multistream



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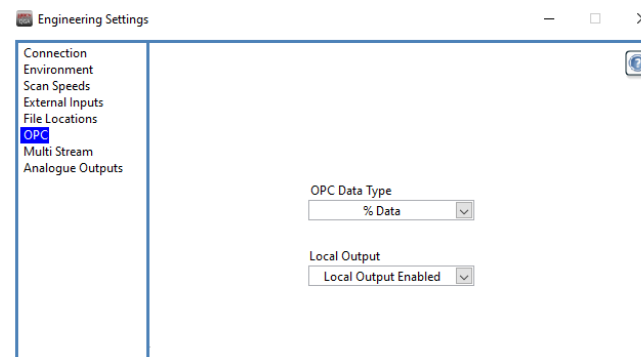
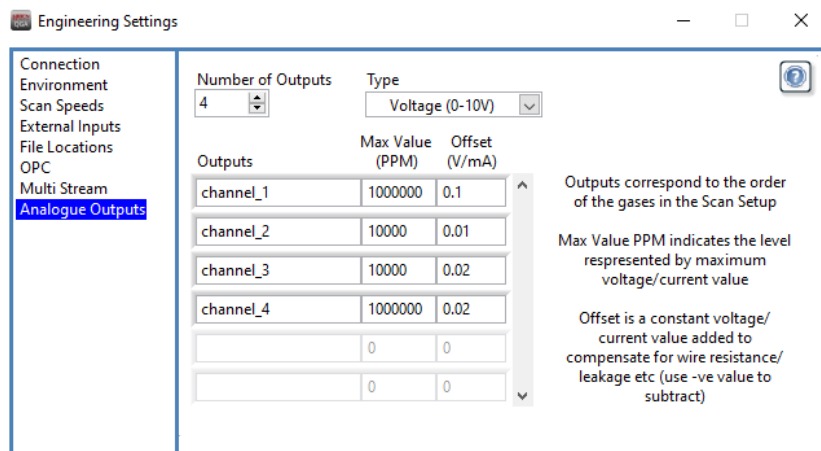
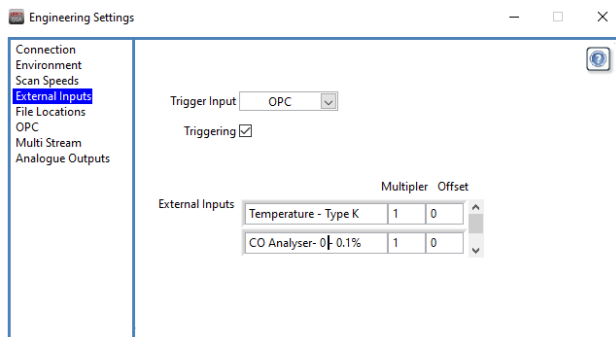
Time (hh:mm:ss)	Stream 1: Oxygen (Corrected (%))	Stream 2: Oxygen (Corrected (%))	Stream 3: Oxygen (Corrected (%))	Stream 4: Oxygen (Corrected (%))	Stream 5: Oxygen (Corrected (%))	Stream 6: Oxygen (Corrected (%))	Stream 7: Oxygen (Corrected (%))	Stream 8: Oxygen (Corrected (%))
00:00:11.64	15.99	15.97	15.91	16.12	16.16	15.93	16.11	15.83
00:00:23.54	15.98	16.21	16.31	16.13	16.26	16.22	16.09	16.14
00:00:35.25	16.08	15.98	15.94	16.06	16.21	15.78	16.11	16.26
00:00:46.84	15.88	16.06	16.10	16.13	16.20	16.11	16.04	16.17
00:00:58.65	15.92	16.16	15.89	16.04	15.89	15.97	15.87	16.01
00:01:10.14	15.86	15.79	15.90	16.18	16.11	16.22	16.14	15.84
00:01:22.05	16.02	16.11	15.76	15.82	15.82	16.17	15.92	15.94

Stream 1
Stream 2
Stream 3
Stream 4
Stream 5
Stream 6
Stream 7
Stream 8

QGA Multi-stream displays up to 4 selected streams on a multi-plot and all selected streams in the tabular view

QGA 2 – External sensors and data export

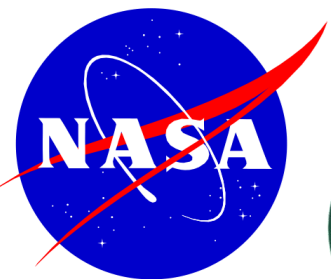
Data from external sensors and devices can be acquired, stored and displayed together with the mass spectrometer data. Analysis start/stop can be controlled via an OPC trigger or from an I/O input/TTL trigger input.



Data is exportable to Excel, and is available to OPC servers through a shared variable engine that publishes data to OPC tags. Data can also be published as analogue outputs in 0-10V or 4-20mA format.

New Features in QGA - 2

- Automatic multiplier voltage optimisation
- Changes to multiplier voltage are effective during analysis
- Scan rate automatically optimised for best signal to noise
- User defined file locations
- Multipoint calibration for accurate quantification over high dynamic range
- Experiment specific fragment ratio assessment
- Spectral simulator for a quick overview of the spectrum with user control to dynamically show changes
- Automatic fragment selection tool based on expected concentration
- Location of overlapping fragments highlighted
- Easy gas position sorting to optimise scan
- Setup file can be created, edited and saved whilst scan is running
- Scan description can be added to setup file
- Real time data smoothing
- Historical data can be viewed during measurement
- Erroneous data point removal option
- Integration of CO analyser data with automatic correction of mass 28 signal
- Export options for background and calibration data, provides full audit of data
- View all streams in single table



The University of Manchester



Delft University of Technology



Johnson Matthey

Hidden QGA Users

Johnson Matthey
Imperial College London

NASA

Poitiers University

Nissan

KTH Stockholm

Karlsruhe Institute of
Technology

University of Florida

The University of Hong
Kong

Paul Scherrer Institut

ULB Brussels University

Texas A&M University

University of Sao Paulo

University College

London

Technical University

Denmark

Beijing Forestry
University

CSIR – Indian Institute of
Petroleum

Diamond Light Source
Shanghai Institute of
Technology

Janssen Pharmaceutica
PDVSA

Air Liquide

BASF

TU Delft

Seoul National University

University of Manchester

University of British

Columbia

USTB

University of Nottingham



Karlsruher Institut für Technologie



BASF
The Chemical Company



AIR LIQUIDE



Summary

- QGA software is designed for use by users with or without experience of mass spectrometry.
- Set-up screens are intuitive and easy to navigate. A calibration wizard guides the user through an automated procedure.
- Raw data, corrected data and quantitative data is acquired, displayed (graphical and tabular formats) and saved in real time.
- Data export on the fly to MS Excel and to tags for OPC compatible clients is included.
- Soft ionisation for reduced spectral fragmentation and simplified data interpretation
- QGA software is offered with Hiden's QIC series gas analysis systems.



- www.HidenAnalytical.com
- The Hiden website is an excellent resource with product pages, brochures, catalogues, product pages with some application notes, presentation and other information.
- Contact +44 1925 445225 for direct support.