



Thermo Fisher Scientific Software Update

María de Castro

GasIRMS Field Applications Specialist EMEA/Global
London, 22-23 September 2023

 The world leader in serving science



Software Releases

- SR 2.15 – Q4 2021
- SR 2.16 – Q3 2022
- SR 2.19 – Q2 2023

Dashboard

ThermoFisher
SCIENTIFIC

Dashboard - Delta Q + GC1310

Configuration Delta Q + GC1310 changed. State changed: Ready

Delta Q Connected ChromControl Connected

Clear Emission and HV ✓ Activate TuneBook CO2 ✓ Turn off Reference Gas ✓ Ready ✓

Instrument Status ConFlo IV

TuneBook

CO2

Intensity Monitor

Channel	Intensity	Offset
CUP 2 X	44	0.001
CUP 3 X	45	0.001
CUP 4 X	46	0.002

Source

- Source:
- High Voltage:
- Trap (mA): 0.62
- Box (mA): 0.88

Analyzer

- High Voltage (kV): 3.852
- Magnet Field (%): 70.643

Heater

- Inlet Valve Heater:
- Source Heater:
- Analyzer Heater:

Vacuum System

- High Vacuum (mbar): 1.23E-006
- Analyzer Turbo Pump > 80%:
- Analyzer Turbo Pump On:
- Main Pump Switch:

Chart Recorder

Intensity (V) vs Time

Time	Intensity (V)
12:15:35	~0.0025
12:15:40	~0.0025
12:15:45	~0.0025
12:15:50	~0.0025
12:15:55	~0.0025
12:16:00	~0.0025
12:16:05	~0.0025
12:16:10	~0.0025
12:16:15	~0.0025

GC Isolink II

HTC Oven

- On: 1200 °C / 1200 °C

Comb Oven

- On: 400 °C / 400 °C

Control

- Backflush (External):
- Backflush (Measure Point): Comb
- Cold Trap:

Conditioning

Mode: Conditioning

Idle

Start Stop

Scheduler

Run [Icons]

Name	Progress	Time Remaining	Information
------	----------	----------------	-------------

Dashboard

- Dashboard
- Instrument
- LabBooks
- Templates
- File Manager
- LabBook Query
- Help

Dashboard - Delta Q + GC1310

Configuration Delta Q + GC1310 changed. State changed: Ready

Clear
Emission and HV ✓
Activate TuneBook CO2 ✓
Turn off Reference Gas ✓
Ready ✓

Delta Q

Connected

ChromControl

Connected

Take Control
Consumables
<Autogenerated>

Thermo Scientific GC Home
Thermo TriPlus RSH
FrontInlet
BackInlet
Oven
Aux Modules and Valves
Audit

SSL Inlet

Status SSL

Inlet type: SSL

		Actual	Setpoint
Carrier pressure:		15.927 [pa]	
Column flow:	<input type="radio"/> On	1.199 [ml/min]	1.200 [ml/min]
Purge flow:	<input type="radio"/> On	5.000 [ml/min]	5.000 [ml/min]
Carrier mode:	<input type="radio"/> On	15.0 [ml/min]	50.0 [ml/min]
Split mode:	<input type="radio"/> On	230 [°C]	230 [°C]

Gas saver: On

Carrier mode: FlowCtrl

Split mode: SplitlessWitl

Column Functions

Column Properties

Leak Check

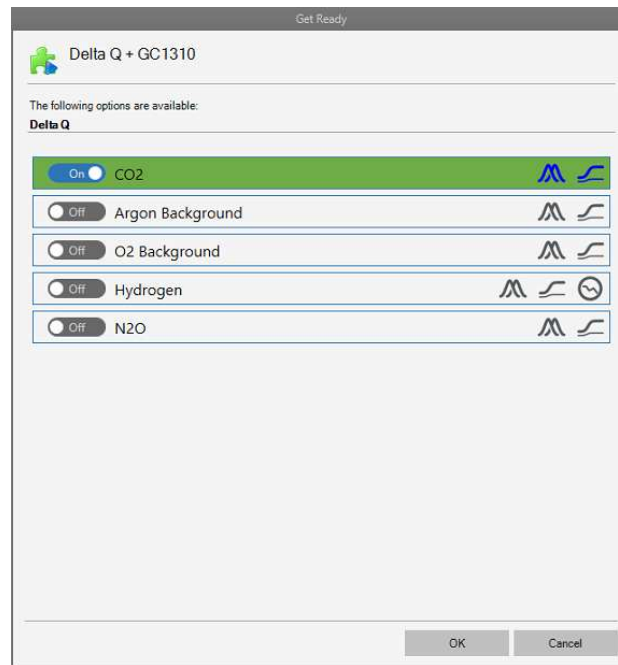
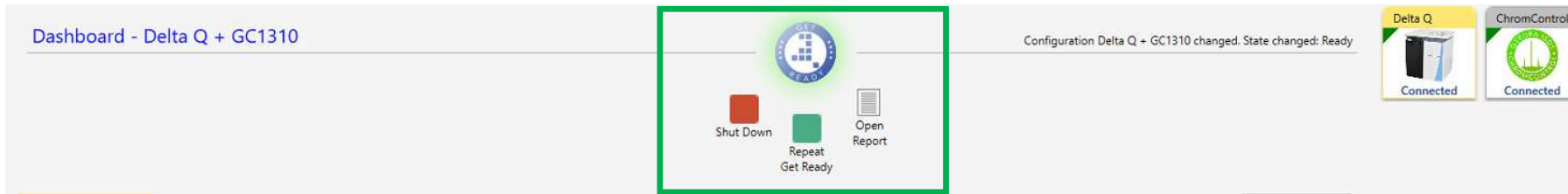
Column Evaluation

	Date	Time	Retention Time	Device	Message
1	9/19/2023	1:15:28 AM +02:00		System	The system time or time zone settings have been changed.
2	9/15/2023	9:13:41 PM +02:00		System	The system time or time zone settings have been changed.
3	9/15/2023	12:48:51 PM +02:00		GC	New detailed run state: Waiting for prep-run key
4	9/15/2023	12:48:51 PM +02:00		GC	Log RunState: StandBy
5	9/15/2023	12:48:27 PM +02:00		TriPlusRSH	Connection established successfully.
6	9/15/2023	12:48:21 PM +02:00		GC	Log Ready: NotReady
7	9/15/2023	12:48:21 PM +02:00		GC	Log RunState: NotReady
8	9/15/2023	12:48:21 PM +02:00		GC	Connection established successfully.
9	9/15/2023	12:48:21 PM +02:00		GC	Log DoorStatus: Closed
10	9/15/2023	12:48:19 PM +02:00		TriPlusRSH	Trying to connect ...
11	9/15/2023	12:48:19 PM +02:00		GC	Trying to connect ...

Scheduler

Run
Progress
Time Remaining
Information

Dashboard \ Get Ready



Instrument



The screenshot displays the 'Instrument' software interface. On the left is a vertical sidebar menu with the following items: Dashboard, Instrument (highlighted in yellow), LabBooks, Templates, File Manager, LabBook Query, and Help. The main content area is titled 'Home' and contains five tool categories, each with an icon and a list of sub-tools:

- Calibrations**: Calibration Tools
- Collectors and Tuning**: Collector Configurator and Tuning
- Diagnostics**: Diagnostic Tools
- Maintenance**: Maintenance Tools
- Factory and Service**: Factory and Service Tools

Instrument \ Calibrations

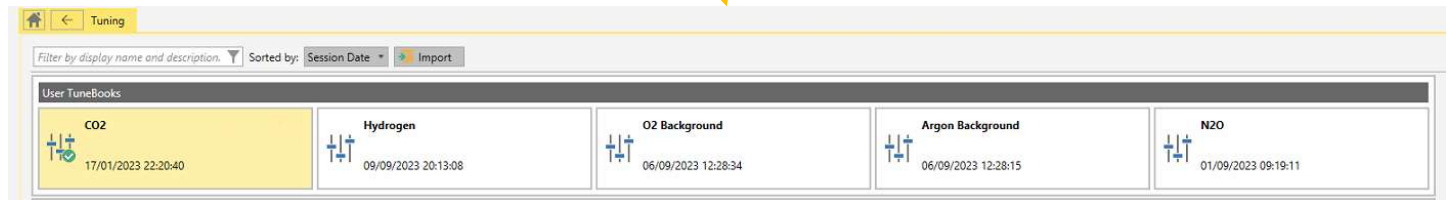
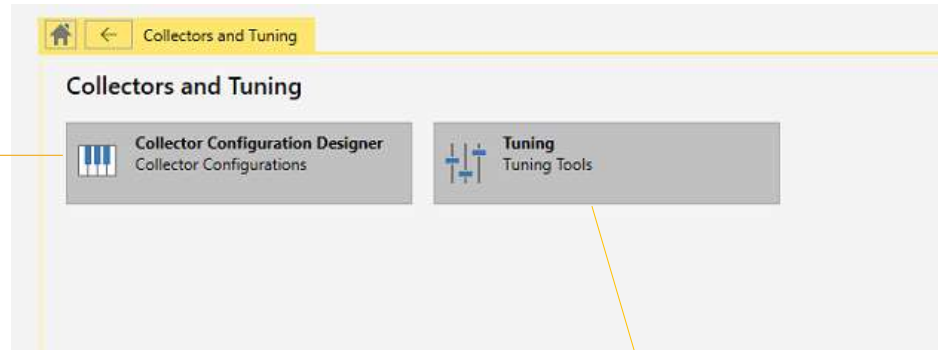
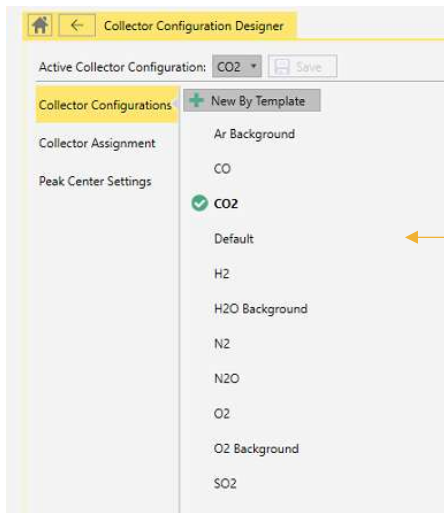


Home < Calibrations

Calibrations

- Mass Calibration
- Electronic Offset Determination
- Jump Calibration
- Reference Gas Calibration

Instrument \ Collectors and Tuning



Instrument \ Collectors and Tuning \ Tuning \ CO₂



- Collector Configuration
- Session History
- Auto Focus
- Manual Focus
- Peak Shape
- Linearity Correction
- Performance Check

Auto Focus

Auto Focus Options

Integration Time: 0.1048576 s Minimum Delay Time: 300 ms

Collector: CUP 2 (CUP 2 Farada) Maximum Delay Time: 500 ms

Minimum Step Width: 1 % Maximum Iterations: 3

Maximum Step Width: 20 % Simulated Poti Turns: 2

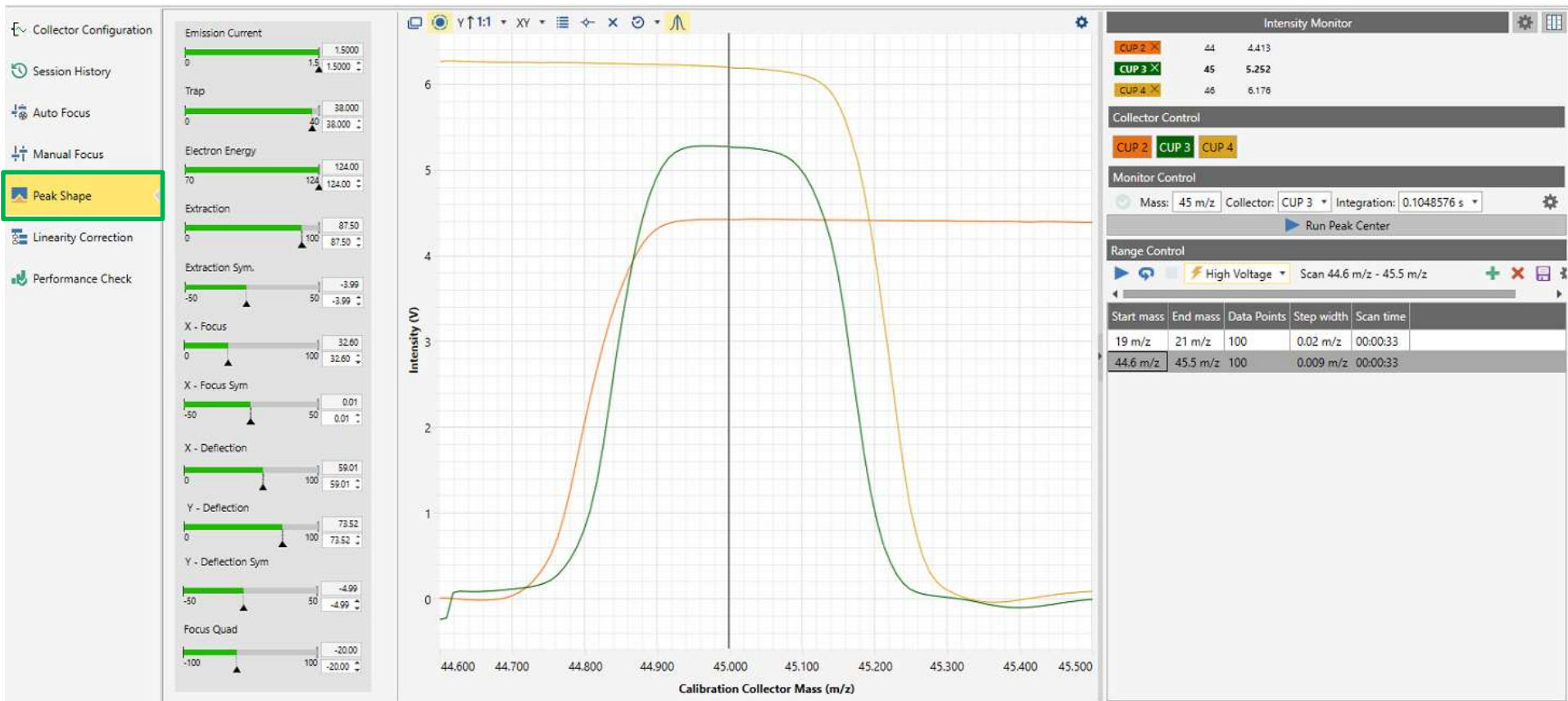
Enabled	Hardware Item
<input type="checkbox"/>	Emission Current Set
<input checked="" type="checkbox"/>	Electron Energy Set
<input checked="" type="checkbox"/>	Trap Set
<input checked="" type="checkbox"/>	Extraction Set
<input checked="" type="checkbox"/>	Extraction Symmetry Set
<input checked="" type="checkbox"/>	X-Focus Set
<input checked="" type="checkbox"/>	X-Focus Symmetry Set
<input checked="" type="checkbox"/>	X-Deflection Set
<input checked="" type="checkbox"/>	Y-Deflection Set
<input checked="" type="checkbox"/>	Y-Deflection Symmetry Set

Auto Focus Parameters

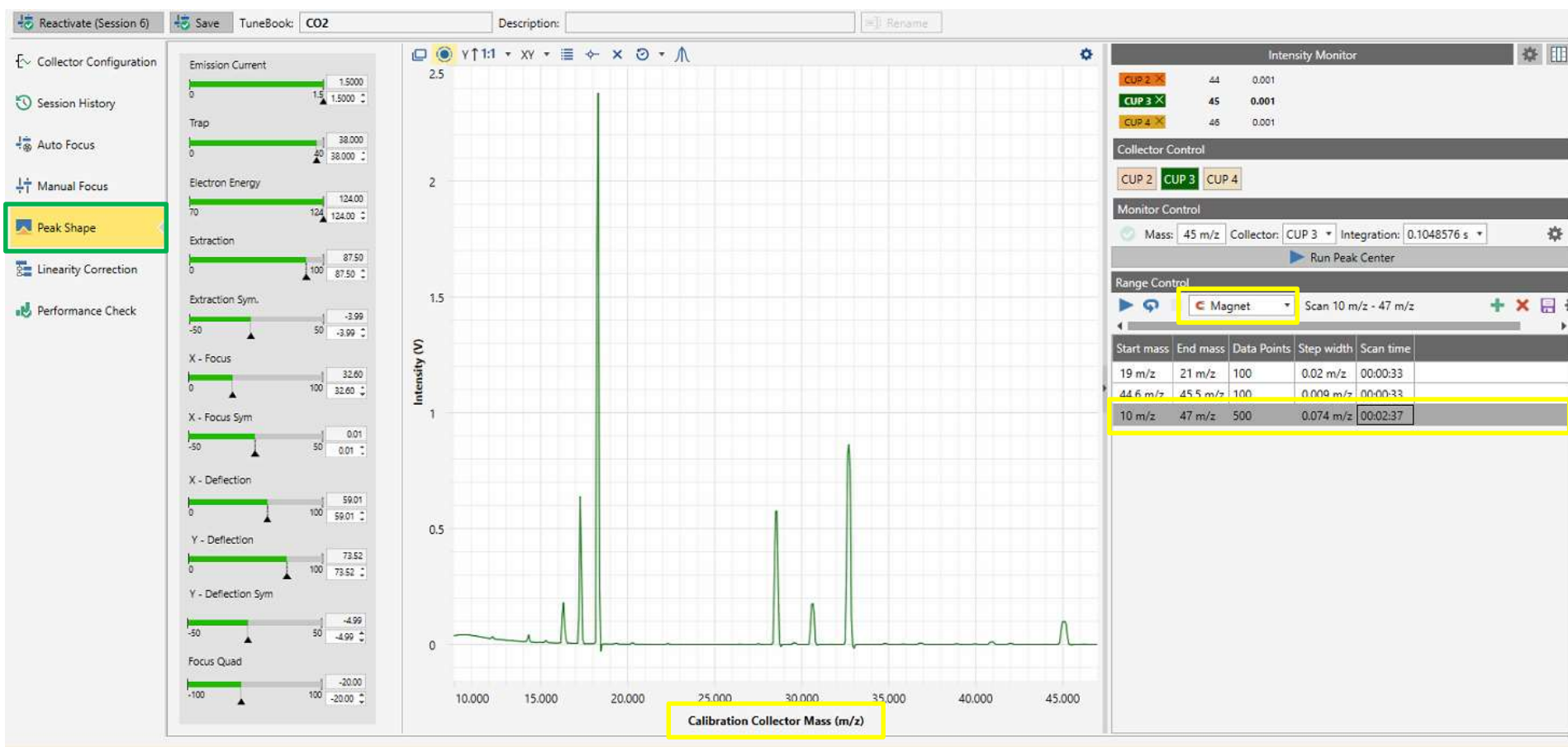
Electron Energy Set	70	84	97	111	124	124.00V
Trap Set	0	10	20	30	40	38.000V
Extraction Set	0	25	50	75	100	87.50%
Extraction Symmetry Set	-50	-25	0	25	50	-3.99%
X-Focus Set	0	25	50	75	100	32.60%
X-Focus Symmetry Set	-50	-25	0	25	50	0.01%
X-Deflection Set	0	25	50	75	100	59.01V
Y-Deflection Set	0	25	50	75	100	73.52%
Y-Deflection Symmetry Set	-50	-25	0	25	50	-4.99%

Auto Focus Progress

Instrument \ Collectors and Tuning \ Tuning \ CO₂



Instrument \ Collectors and Tuning \ Tuning \ CO₂



Instrument \ Diagnostics

Home < Diagnostics

Diagnostics

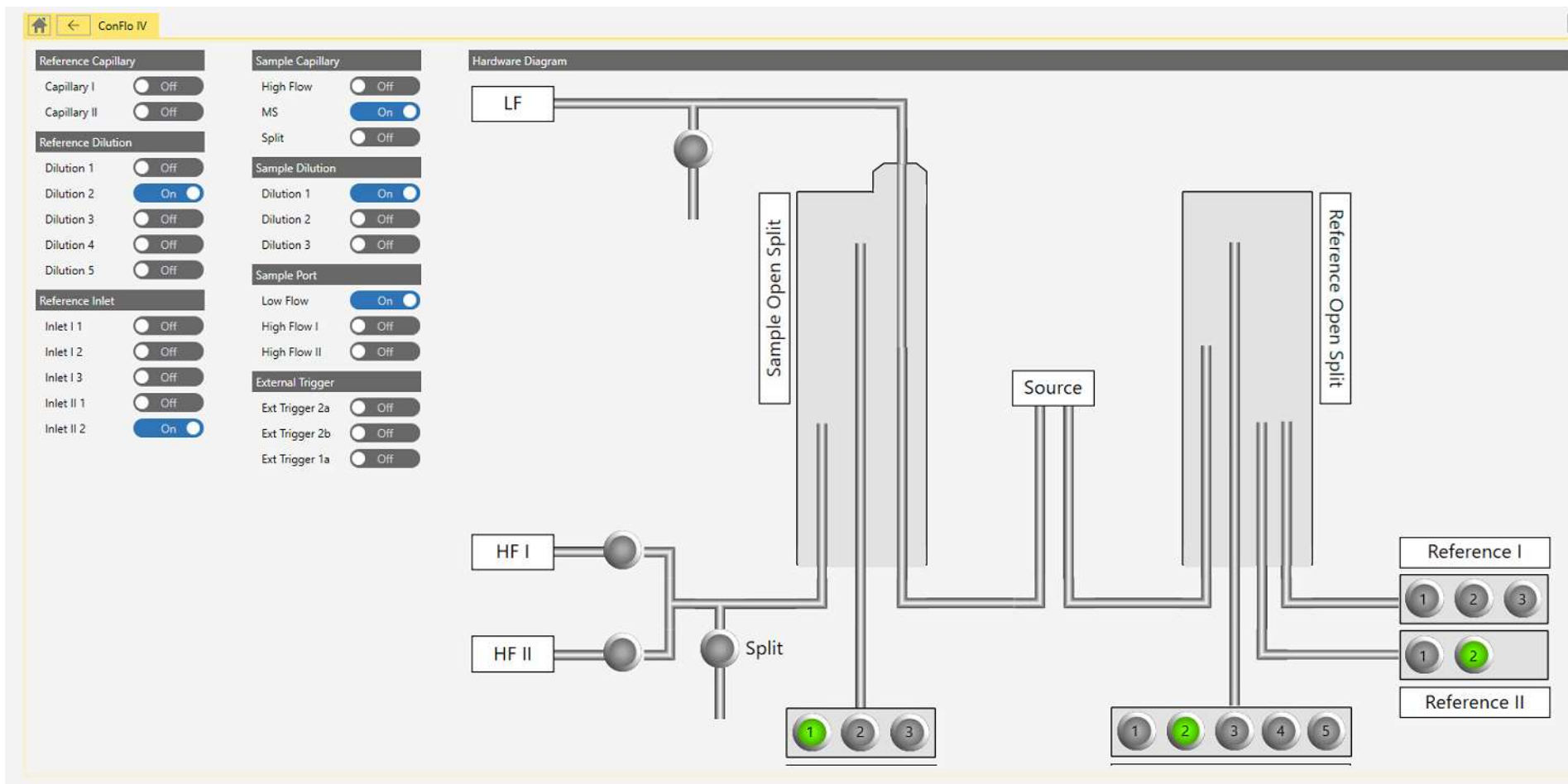
- Mass Spectrometer**
Diagnostic details panel for the Mass Spectrometer
- ConFlo IV**
- GC Isolink II**
- Chart Data Importer**
Import and present saved chat data

The diagnostic panel for the Mass Spectrometer features several control elements:

- Magnet Field (%)**: Slider from 0 to 100, current value 70.643.
- High Voltage (kV)**: Slider from 0 to 3.3, current value 3.0518.
- Emission Current**: Slider from 0 to 1.5, current value 1.5000.
- Source**: On/Off toggle, currently On.
- High voltage (kV)**: On/Off toggle, currently On.
- High Vacuum (mbar)**: Value 1.22E-006.
- Trap (mA)**: Input field with value 0.62.
- Box (mA)**: Input field with value 0.88.
- Trap**: Slider from 0 to 38.000, current value 38.000.
- Electron Energy**: Slider from 70 to 124, current value 124.00.
- Extraction**: Slider from 0 to 100, current value 87.50.
- Extraction Sym.**: Slider from -50 to 50, current value -3.99.
- X - Focus**: Slider from 0 to 100, current value 32.60.
- X - Focus Sym**: Slider from -50 to 50, current value 0.01.
- X - Deflection**: Slider from 0 to 100, current value 59.01.
- Y - Deflection**: Slider from 0 to 100, current value 73.52.
- Y - Deflection Sym**: Slider from -50 to 50, current value -4.99.
- Focus Quad**: Slider from -100 to 100, current value -20.00.

CAUTION!
This panel is for diagnostic use by trained personnel only.
Be aware that wrong handling can cause hardware damage or unwanted changes in active TuneBook.
If the magnet field is changed here, keep in mind that the new state could deviate from the set value due to the hysteresis effect. Use Get Ready to load another TuneBook and achieve a complete magnet reset if necessary.

Instrument \ Diagnostics \ ConFlo IV



Instrument \ Diagnostics \ GC Isolink II

The screenshot displays the GC Isolink II diagnostic interface, organized into several functional areas:

- Control Panel (Left):**
 - Backflush Ext Heater:** On
 - Valves:**
 - Backflush (External): On
 - Backflush (Measure Point): Off
 - Flow Meter: Off
 - O2: Off
 - CH4: Off
 - Vent: Off
 - He: On
 - 4 Port: On
 - Cold Trap: Off
 - Status:**
 - GC Start Active: Off
 - HTC Oven On: On
 - Comb Oven On: On
 - Backflush Overheated: Off
 - Power State Error: Off
 - HTC Temp Sensor Error: Off
 - Comb Temp Sensor Error: Off
 - HTC Short Circuit: Off
 - HTC Open Circuit: Off
 - Comb Short Circuit: Off
 - Comb Open Circuit: Off
 - Overheated: Off
 - Error Flag: Off
 - Software Toggle: Off
- HTC Oven (Top Middle):**
 - State: On
 - Temp: 1200.0 °C (setpoint), 1200.1 °C (actual)
 - Current: 16.6 A (setpoint), 7.9 A (actual)
- Comb Oven (Middle Middle):**
 - State: On
 - Temp: 400.0 °C (setpoint), 399.7 °C (actual)
 - Current: 12.5 A (setpoint), 1.2 A (actual)
- Internal Flowmeter (Bottom Middle):**
 - Graph showing Flow (ml/min) vs Time. The flow is stable at approximately 0.1 ml/min.
 - Time range: 13:02:00 to 13:06:00.
- Hardware Diagram (Right):**
 - Shows the physical layout of the instrument with components like Flow Meter, Measure point, Ovens (Combustion Oven at 400°C and HTC Oven at 1200°C), Gas Supply (O2, CH4, He, N2), and Vent.
 - Includes an External Backflush Heater and a Water Removal trap.
- Tools (Bottom Right):**
 - Straight
 - Backflush
 - Conditioning Combustion
 - Conditioning HTC

LabBooks

LabBooks

Create LabBook
Create a new LabBook based on an existing Template or LabBook

Name: 33-2_13C_SSL back_10ul syringe - 230923 - Classic Method 1.5mlmin

Location: LabBooks\Delta Q + Trace GC + RSH\2023\Apr_2023\20230410 33-2 classic

Create a new LabBook from an existing Template

Template Name: [dropdown] [...]

Samples: 1 Import from CSV

CSV name: [dropdown] [...]

Mapping Name: [dropdown] [...]

Create a new LabBook from an existing LabBook

LabBook Name: 33-2_13C_SSL back_10ul syringe - 010042023 - Classic Method 1.5mlmin

Create a new LabBook from a blank Template

Evaluation: Qtegra™ IsoScale G

Create LabBook

Open LabBook
Open an existing LabBook

Open...

Browse for LabBook

Delta Q + Trace GC + RSH > 2023 > Apr_2023

Create New Folder Views

- Delta Q + Gas Bench + Precon + RSH
- Delta Q + GB + Precon
- Delta Q + GB + RSH
- Delta Q + GC Isolink
- Delta Q + Trace GC + RSH
 - 2022
 - 2023
 - Apr_2023
 - 20230401 33-2 GC Isolink II reac
 - 20230402 Steroids
 - 20230403 Steroids
 - 20230404 Steroids 33-2 classic
 - 20230405 33-2 classic_90mins o
 - 20230406 33-2 classic
 - 20230407 33-2 classic
 - 20230408 33-2 classic
 - 20230409 33-2 J01
 - 20230410 33-2 classic
 - 20230411 33-2 classic_90mins o

Name

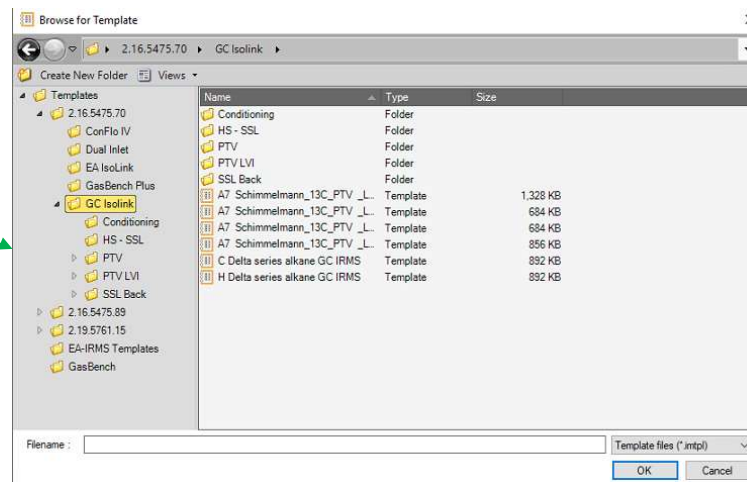
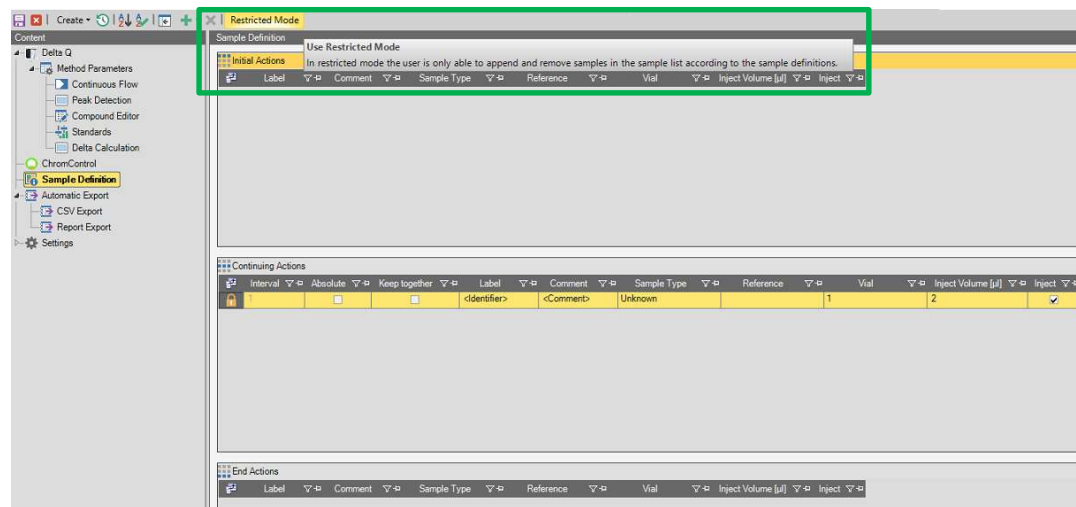
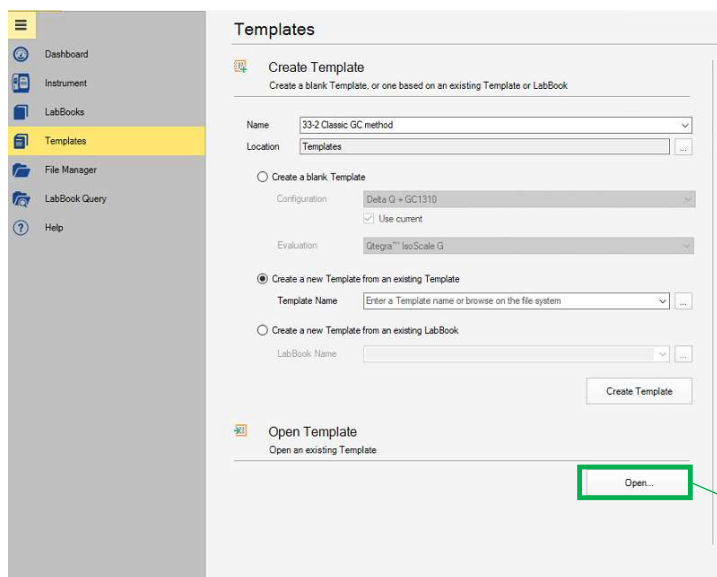
- 20230403 Steroids
- 20230404 Steroids 33-2 classic
- 20230405 33-2 classic_90mins oxid
- 20230406 33-2 classic
- 20230407 33-2 classic
- 20230408 33-2 classic
- 20230409 33-2 J01
- 20230410 33-2 classic
- 20230411 33-2 classic_90mins oxid
- 20230413 HD Alkanes SSL
- 20230414 HD A7 SSL
- 20230415 HD A7 SSL
- 20230417 Cetona
- 20230418 Cetona
- 20230419 Cetona
- 20230420 Cetona
- 20230421 Cetona-new SGE T- 3hs oxid
- 20230422 Cetona
- 20230423 Cetona

Filename: [text field]

LabBook files (*.inexp)

OK Cancel

LabBookTemplates



LabBook \ Continues Flow and Peak Detection

Continuous Flow (CO2)

Instrument

TuneBook: CO2 | Linearity: On

Integration Time: 0.2097192 s | Start at Sample: 1

Peak Center: On | Interval: 50

Peak Center For First Gas Only: No

Peripheral Parameters

GC Isolink II

Conditioning: On

Start at Sample: 1 | with: Extended

Interval: 40 | Seed: 1

Timeline

- Backflush (Measure Point): 1 s, State: On
- Referencing: 30 s, Number of Pulses: 10, Pulse Width: 20 s, Dilution: Target Intensity, Interval: 30 s
- Backflush (Measure Point): 500.0 s

Estimated sample runtime: 00:30:00

Peak Detection

Measure Line Peak Finder Parameters

CO2 Traces: 44.00 m/z, 45.00 m/z, 46.00 m/z

Detection Trace: 44.00 m/z

Segments

+ Add | Parameter Set (Start - End)

Parameter Set (Start - End)

Name: Parameter Set

Evaluation Range

From Start: Auto | To End: Auto

Time Shift Settings

Perform Time Shift: On | Extended Time Shift: Off | Maximum Time Shift: 0.5 s

Slope Settings

Number of Slope Data Points: 5

Start Slope: 0.002 V/s | Top Slope: 5E-05 V/s | End Slope: 0.002 V/s

Peak Limits

Maximum Peak Width: 180 s | Minimum Peak Height: 0.005 V | Peak Limit to Ampl.: 0 % | Peak Resolution: 20 %

Square Peak Settings

Square Pulse Detection Fraction: 0.55

Post Filter Settings

Use Post Filter: On | Maximum Peak Width: 180 s | Minimum Peak Height: 0.25 V

Background Settings

Background Type: Individual | Number of Background History Points: 25 | Smooth Type: Standard | Number of Smoothing Data Points: 5

LabBook \ Compound Editor – Drift Correction

The screenshot displays the Compound Editor interface. On the left is a navigation tree with 'Compound Editor' selected. The main window has a 'Time Unit (Seconds / Minutes)' toggle set to 's'. Below it is a table of compounds with their retention times and tolerances.

Name	Retention Time (s)	Tolerance (s)
5a-an-ac	743.2	10
Cholestane	1068.2	10
Andro-ac	896.0	10
11 Keto-ac	948.4	10

The 'Drift Correction Compound Name' dropdown is set to 'None', with a list of options including '5a-an-ac', 'Cholestane', 'Andro-ac', and '11 Keto-ac'.

A 'Load Compounds' dialog is open, showing a 'Compound Library' and a 'Current Compound Set'.

Identifier	Description
BTEX	
BTEX TG624	
BTEX + MeOH TG624	
BTEX Schimmelmann	
Indiana Mix A7	
Indiana Mix A7 - 03	
Indiana Mix A7 - Aux Gas	
Indiana Mix A7 70C	
Indiana Mix A7 PTV Front	
Indiana Mix A7 SSL - 03	
Indiana Mix A7 SSL 11012023 - 02	
Indiana Mix A7 SSL 12012023	
Indiana Mix A7 SSL 12012023-01	
Indiana PAHs N-P- US method	

Name	Retention Time (s)	Tolerance (s)
Benzene	298.0	10
Ethylbenzene	375.0	10
Toluene	454.0	10
o-Xylene	535.0	5
p-Xylene	543.0	5
m-Xylene	572.0	10

LabBook \ Standards and Delta Calculation Parameters

Standards

Name	Description
CU/PCC 33-2	Derivatized Steroids
CO2 UAM	

Selected Compound(s) for "CU/PCC 33-2"

Compound
5a-an-ac
Cholestane
Andro-ac
11 Keto-ac

Selected Delta(s) for "Andro-ac"

Delta Identifier	Delta Value (%)	Primary Standard	Primary Standard Ratio
13C	-32.58	VPDB 13C/12C	0.0111802
18O	0	VSMOW 18O/16O	0.0020052

Standard Library

Select Standards you want to import.

Type	Name	Description
CO2 UAM		
Indiana Mix B3		GC-IRMS
Alkane Mix C14-C16		GC-IRMS
CO2		PreCon GC-IRMS
N2O		PreCon GC-IRMS
BTX Schimmelmann		Schimmelmann Certifi
Schimmelmann A7		
Schimmelmann A7 HTC		
PAHs Schimmelmann		Indiana Naphthalene
Indiana PAHs + m - Xylene		Schimmelmann Certifi
A7 + PAHs Mix Schimmelmann		A7 + Naphthalene + P
34-3		CUPCC
MXD18-1		NMI
MXD18-2		CUPCC
Schimmelmann A7 + PAHs HTC		
F8-4 Indiana		FAMES
FAMES Mix UAM		
Schimmelmann B5		
CU/PCC 33-2		Derivatized Steroids

Selected Compound(s) for "CU/PCC 33-2"

Compound
5a-an-ac
Cholestane
Andro-ac
11 Keto-ac

Selected Delta(s) for "Andro-ac"

Delta Identifier	Delta Value (%)	Primary Standard	Prim
13C	-32.58	VPDB 13C/12C	0.01
18O	0	VSMOW 18O/16O	0.00

Delta Calculation Parameters

CO₂ (Brand, Assonov & Coplen, 2010)

Standard Name: CO2 UAM

R45: 45C.O./44C.O.O.

R46: 46C.O./44C.O.O.

Reference Peak: 10

GC Limits:

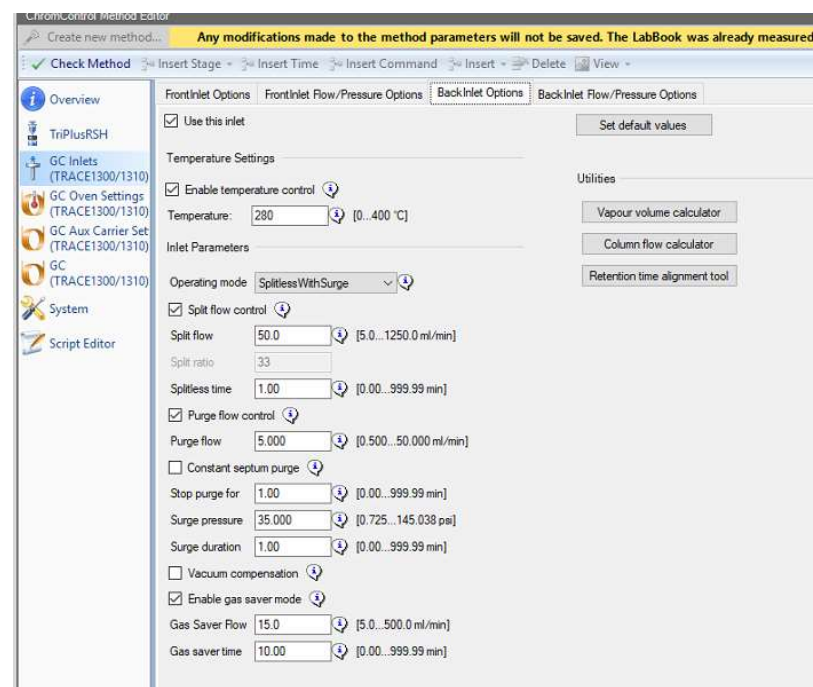
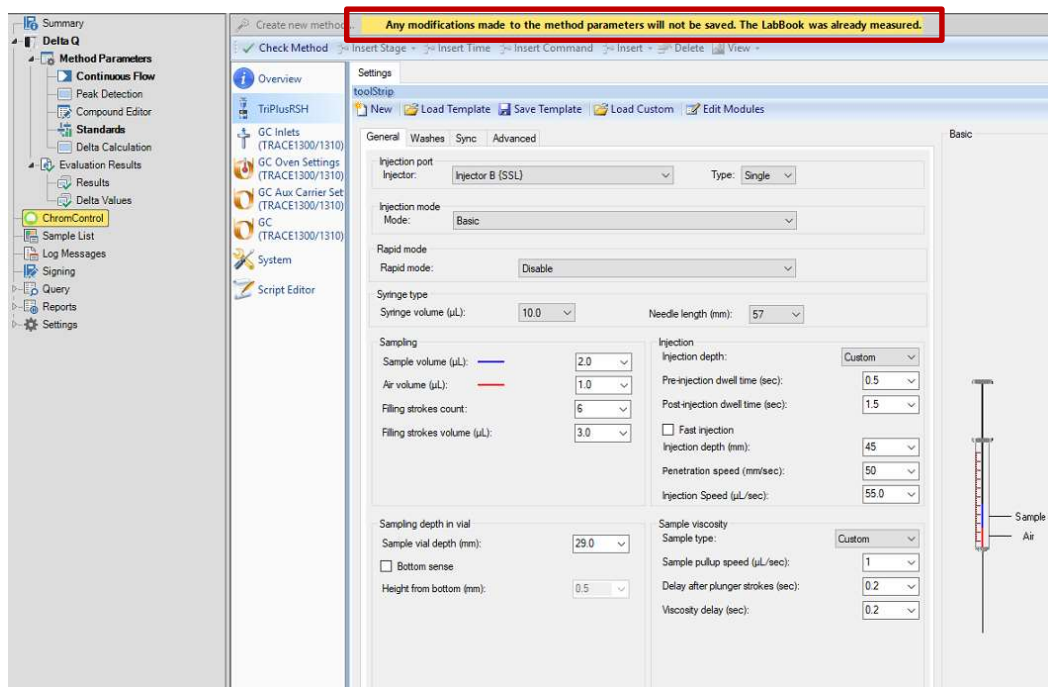
- d13: 2, 3, 4, 5, 6, 7, 8, 9, 10
- d18: 2, 3, 4, 5, 6, 7, 8, 9, 10

Ratio Converter:

- ¹⁸O - correction: 0.01022444
- K (constant): 0.528
- α (fractionation factor):

Autosampler and GC Methods: Chromcontrol

- Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software integration

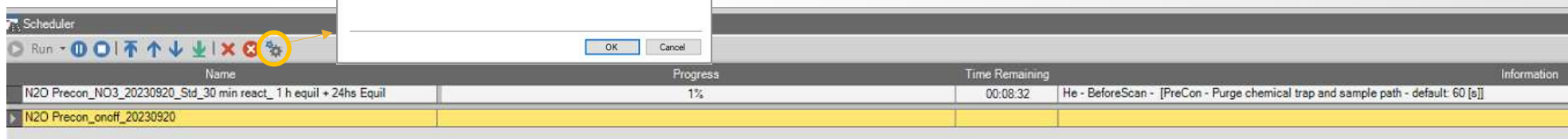
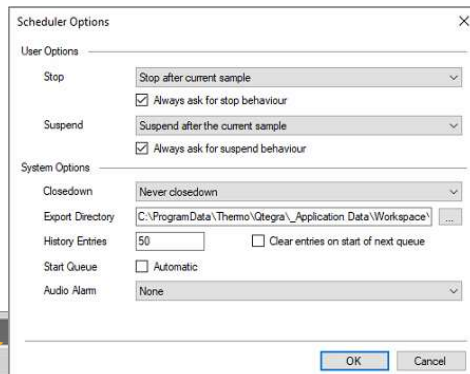
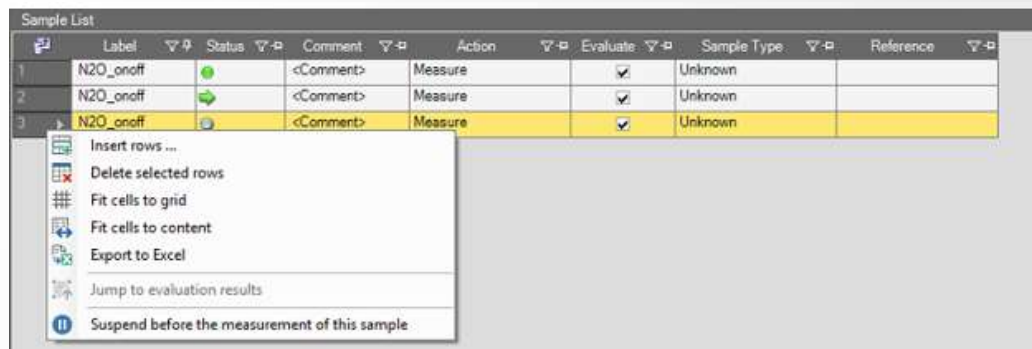
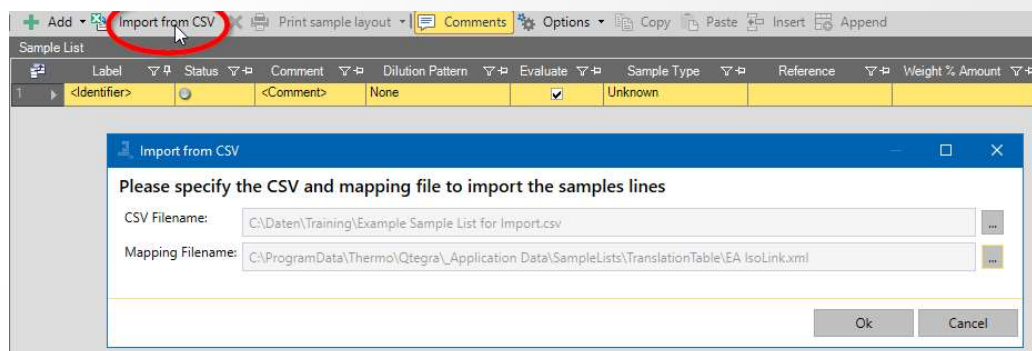


LabBook \ Sample List

Sample List											
	Label	Status	Comment	Run ID	Evaluate	Sample Type	Reference	Vial	Inject Volume [μl]	Inject	
1	Solvent	●		1	✓	Unknown		54	10	✓	
2	MX018-1	●	5 ngul	2	✓	Delta Standard (CSIA)	MX018-1	20	10	✓	
3	MX018-1	●	5 ngul	3	✓	Unknown		20	10	✓	
4	MX018-1	●	5 ngul	4	✓	Unknown		20	10	✓	
5	MX018-1	●	5 ngul	5	✓	Unknown		20	10	✓	
6	MX018-2	●	5 ngul	6	✓	Unknown		21	10	✓	
7	MX018-2	●	5 ngul	7	✓	Unknown		21	10	✓	
8	MX018-2	●	5 ngul	8	✓	Unknown		21	10	✓	
9	Solvent	●		9	✓	Unknown		53	10	✓	
10	Solvent	●		10	✓	Unknown		53	10	✓	
11	F1_QCN_11-Keto	●		11	✓	Unknown		1	10	✓	
12	F2_QCN_Testo	●		12	✓	Unknown		2	10	✓	
13	F3_QCN_11-EpiT	●		13	✓	Unknown		3	10	✓	
14	F4_QCN_5b-diol	●		14	✓	Unknown		4	10	✓	
15	F5_QCN_5a-diol	●		15	✓	Unknown		5	10	✓	
16	F6_QCN_PD	●		16	✓	Unknown		6	10	✓	
17	MX018-1	●	5 ngul	17	✓	Unknown		20	10	✓	
18	MX018-2	●	5 ngul	18	✓	Unknown		21	10	✓	
19	F1_QCP_11-Keto	●		19	✓	Unknown		7	10	✓	
20	F2_QCP_Testo	●		20	✓	Unknown		8	10	✓	
21	F3_QCP_11-EpiT	●		21	✓	Unknown		9	10	✓	
22	F4_QCP_5b-diol	●		22	✓	Unknown		10	10	✓	
23	F5_QCP_5a-diol	●		23	✓	Unknown		11	10	✓	
24	F6_QCP_PD	●		24	✓	Unknown		12	10	✓	
25	MX018-1	●	5 ngul	25	✓	Unknown		20	10	✓	
26	MX018-2	●	5 ngul	26	✓	Unknown		21	10	✓	

LabBook \ Sample List – Sequence Scheduler

- Import/Export Sample Lists (CSV)
- Edit the sample list when it's already running
 - Add/remove injections
 - Partial sequence
 - Change injection volumen
 - Add/modify comments
 - Change Sample Type and/or Reference standard
 - Change vial position



LabBook \ Sample List

Sample List											
	Label	Status	Comment	Run ID	Evaluate	Sample Type	Reference	Vial	Inject Volume [µl]	Inject	
1	Solvent	●		1	☑	Unknown		54	10	☑	
2	MX018-1	●	5 ngul	2	☑	Delta Standard (CSIA)	MX018-1	20	10	☑	
3	MX018-1	●	5 ngul	3	☑	Unknown		20	10	☑	
4	MX018-1	●	5 ngul	4	☑	Conditioning		20	10	☑	
5	MX018-1	●	5 ngul	5	☑	Delta Standard (CSIA)		20	10	☑	
6	MX018-2	●	5 ngul	6	☑	Drift Correction		21	10	☑	
7	MX018-2	●	5 ngul	7	☑	QC Standard		21	10	☑	
8	MX018-2	●	5 ngul	8	☑	Ref Gas Calibration		21	10	☑	
9	Solvent	●		9	☑	Unknown		53	10	☑	
10	Solvent	●		10	☑	Unknown		53	10	☑	
11	F1_QCN_11-Keto	●		11	☑	Unknown		1	10	☑	

Sample List											
	Label	Status	Comment	Run ID	Evaluate	Sample Type	Reference	Vial	Inject Volume [µl]	Inject	
1	Solvent	●		1	☑	Unknown		54	10	☑	
2	MX018-1	●	5 ngul	2	☑	Delta Standard (CSIA)	MX018-1	20	10	☑	
3	MX018-1	●	5 ngul	3	☑	Unknown		20	10	☑	
4	MX018-1	●	5 ngul	4	☑	Unknown	34-3	20	10	☑	
5	MX018-1	●	5 ngul	5	☑	Unknown	MX018-1	20	10	☑	
6	MX018-2	●	5 ngul	6	☑	Unknown	MX018-2	20	10	☑	
7	MX018-2	●	5 ngul	7	☑	Unknown		21	10	☑	
8	MX018-2	●	5 ngul	8	☑	Unknown		21	10	☑	
9	Solvent	●		9	☑	Unknown		53	10	☑	

Data Normalization (External Referencing)



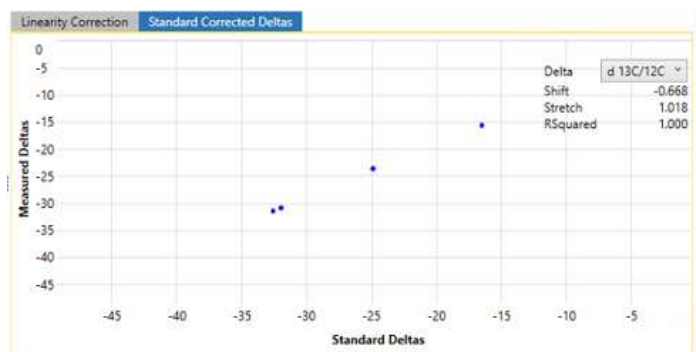
Drift Correction (Time correction)

Compound Editor

Add New Load... Save... Time Unit (Seconds / Minutes)

Name	Retention Time (s)	Tolerance (s)
5a-an-ac	743.2	10
Cholestane	886.2	10
Andro-ac	922.7	10
11 Keto-ac	1001.9	10

Drift Correction Compound Name: 5a-an-ac

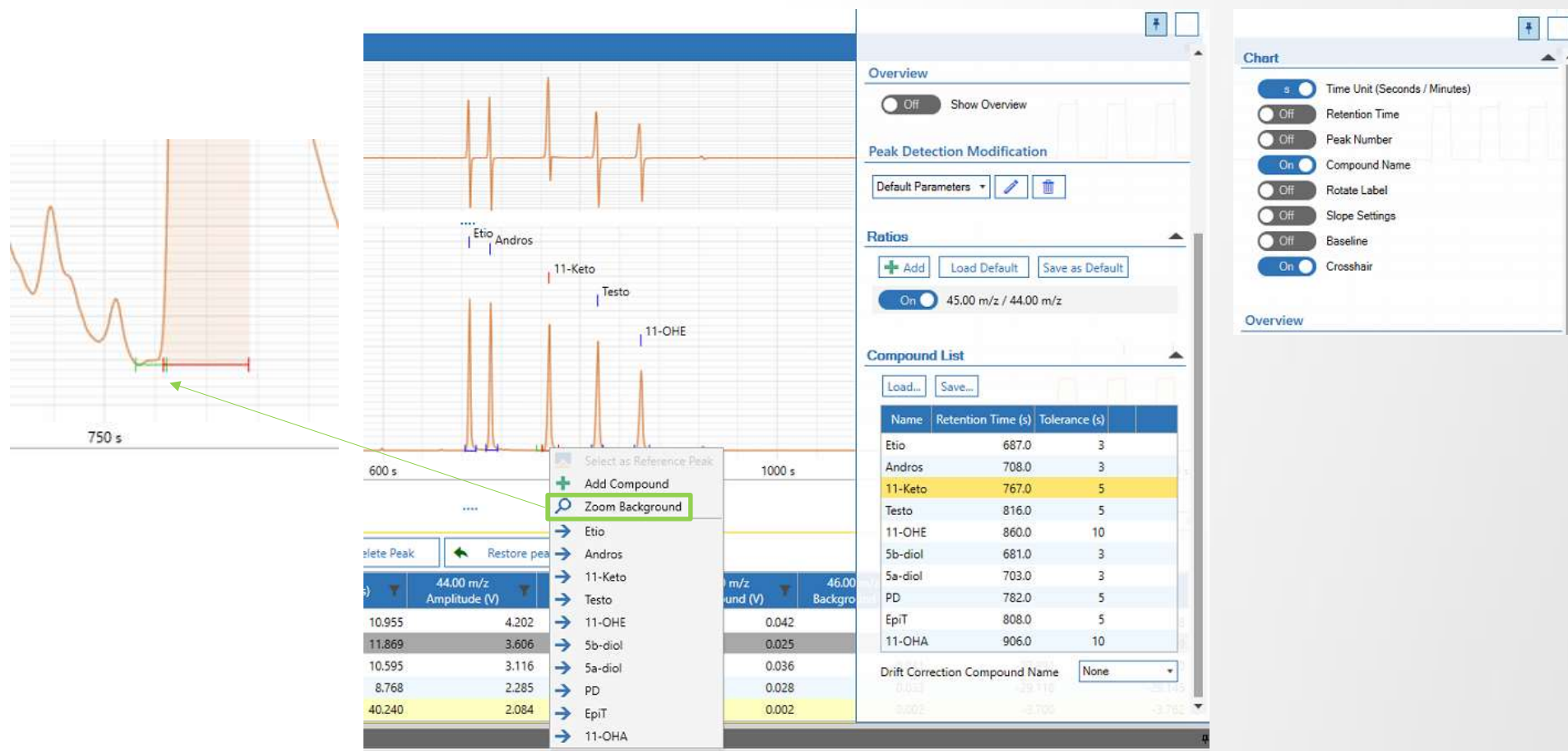


Sample List

	Label	Status	Comment	Run ID	Evaluate	Sample Type	Reference	Vial	Inject Volume (µl)	Inject
1	EtAc	●		1	✓	Unknown		53	2	✓
2	EtAc	●		2	✓	Unknown		53	2	✓
3	33-2	●	10 ngul	3	✓	Drift Correction		1	2	✓
4	33-2	●	10 ngul	4	✓	Delta Standard (CSIA)	CU/PCC 33-2	1	2	✓
5	33-2	●	10 ngul	5	✓	Unknown		1	2	✓
6	33-2	●	10 ngul	6	✓	Unknown		1	2	✓
7	33-2	●	10 ngul	7	✓	Unknown		1	2	✓
8	33-2	●	10 ngul	8	✓	Unknown		1	2	✓
9	33-2	●	10 ngul	9	✓	Unknown		1	2	✓
10	33-2	●	10 ngul	10	✓	Unknown		1	2	✓
11	33-2	●	10 ngul	11	✓	Unknown		1	2	✓
12	33-2	●	10 ngul	12	✓	Unknown		1	2	✓
13	33-2	●	10 ngul	13	✓	Unknown		1	2	✓
14	33-2	●	10 ngul	14	✓	Drift Correction		1	2	✓
15	EtAc	●		15	✓	Unknown		53	2	✓

Peak	Retention Time (s)	Width (s)	Total Area (Vs)	44.00 m/z Amplitude (V)	44.00 m/z Background (V)	45.00 m/z Background (V)	46.00 m/z Background (V)	d 13C/12C	d 13C/12C (ext. ref.)	d 13C/12C (drift corr.)
Peak 13	631.0	24.0	43.357	2.234	0.034	0.059	0.044	-3.142	-3.924	-3.219
Peak 14	706.0	24.0	43.229	2.233	0.031	0.035	0.040	-3.177	-3.959	-3.253
(15) 5a-an-ac	744.5	17.6	4.993	1.512	0.035	0.040	0.045	-30.748	-32.034	-30.825
(16) Cholestane	887.2	16.7	5.482	1.642	0.056	0.066	0.074	-23.898	-25.058	-23.974
(17) Andro-ac	924.0	15.9	4.497	1.289	0.069	0.080	0.091	-31.511	-32.810	-31.588
(18) 11 Keto-ac	1003.2	19.9	4.159	1.001	0.068	0.079	0.090	-15.616	-16.625	-15.692

Data Visualization



Data Visualization

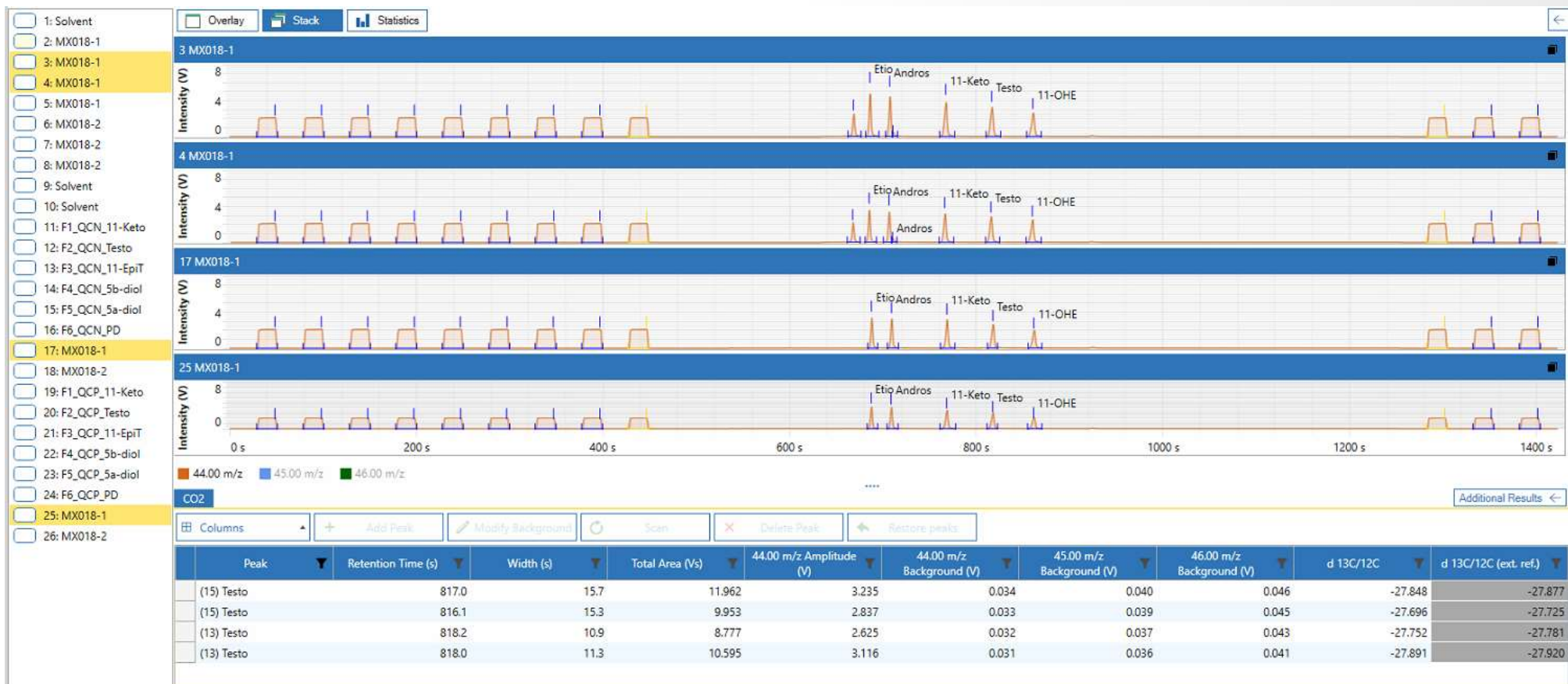
Stacked and overlaid chromatogram view = better insight for method development



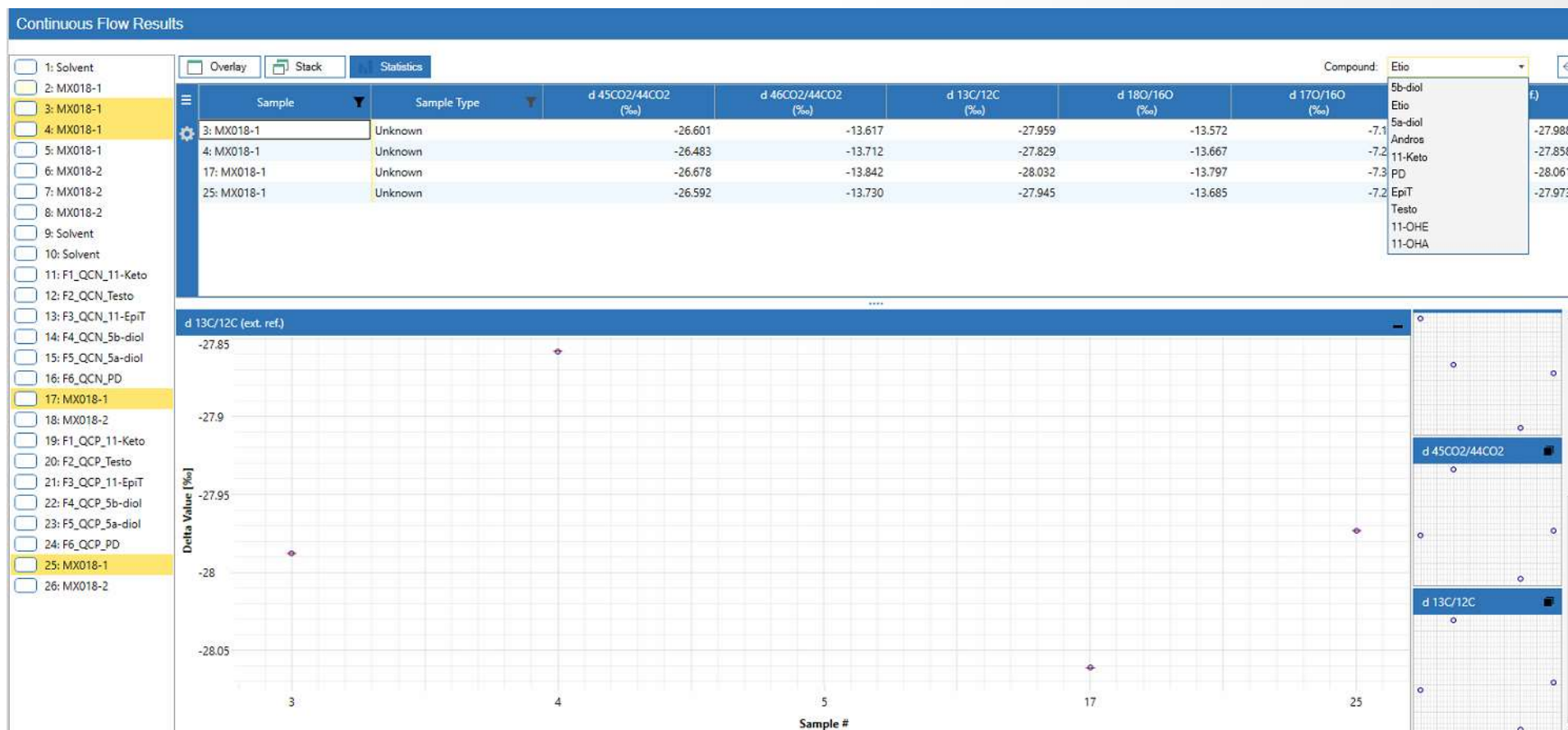
Data Visualization



Data Visualization



Data Visualization



Data Export

Home Page Steroids_13C_PTV_LVI_DB35MS_AuxGas inGC - Sintered liner - 25ul - 20230201 - KCL - B01 - QCs

Export 'Steroids_13C_PTV_LVI_DB35MS_AuxGas inGC - Sintered liner - 25ul - 20230201 - KCL - B01 - QCs' (Ctrl+E)

Exports the data from 'Steroids_13C_PTV_LVI_DB35MS_AuxGas inGC - Sintered liner - 25ul - 20230201 - KCL - B01 - QCs'

Run	Label	Sample Type	Value	Unit	Value	Unit	Value	Unit	Value	Unit	Value	Unit	CO2Bac d13	CO2Bac d13 ext. ref.
31	18	MX018-1	ChromReference	18	1352.4390016	s	22.5719936000000042	s	2.1043414149375907	V	40.143974685844462	Vs	-3.6744578912948356	%
32	19	MX018-1	ChromReference	19	1402.3899904	s	22.3629952000000114	s	2.1096338992423176	V	40.237428778763437	Vs	-3.7609456105711647	%
33	1	MX018-1	Unknown	1	48.6969884	s	22.5719936000000003	s	2.1137478194263437	V	40.192122743682958	Vs	-3.5440284628400764	%
34	2	MX018-1	Unknown	2	98.648	s	22.5720063999999992	s	2.1147475169630621	V	40.322044835257735	Vs	-3.7107321305968055	%
35	3	MX018-1	Unknown	3	148.3900032	s	22.5720064000000021	s	2.1134525800488708	V	40.3120758193663	Vs	-3.733374670355683	%
36	4	MX018-1	Unknown	4	198.1320064	s	22.3629952	s	2.1160129917082493	V	40.331180651301374	Vs	-3.7815638600505741	%
37	5	MX018-1	Unknown	5	247.8740096	s	22.5719936000000013	s	2.1096585346832968	V	40.271401801626268	Vs	-3.8113915777348017	%
38	6	MX018-1	Unknown	6	297.616	s	22.571993599999985	s	2.1097344488958306	V	40.235983711968757	Vs	-3.8012454081792768	%
39	7	MX018-1	Unknown	7	347.3580032	s	22.5720064000000021	s	2.1076514242771887	V	40.209257176453136	Vs	-3.8164175811088441	%
40	8	MX018-1	Unknown	8	397.1000064	s	22.5720064000000021	s	2.1098815347593662	V	40.209175389503322	Vs	-3.8586253989204566	%
41	9	MX018-1	Unknown	9	446.8420096	s	22.3629952	s	2.1089848077489513	V	40.250328215062694	Vs	-3.7	%
42	10	MX018-1	Unknown	10	668.8	s	14.002995199999987	s	2.5024331887579097	V	6.5476439531591826	Vs	-28.363534678758629	%
43	11	MX018-1	Unknown	11	686.3560064	s	14.212006399999995	s	4.7522837612124365	V	11.75211527130377	Vs	-27.98958875616783	%
44	12	MX018-1	Unknown	12	707.6740096	s	7.3149951999999985	s	4.4493447715718268	V	11.220456626283002	Vs	-27.777027456627579	%
45	13	MX018-1	Unknown	13	711.0180096	s	5.6430080000000089	s	0.4339968496379696	V	0.961699481614554	Vs	-32.98264455443389	%
46	14	MX018-1	Unknown	14	767.6569884	s	16.301990400000022	s	3.7963876144467008	V	12.699624015797934	Vs	-13.589334611760485	%
47	15	MX018-1	Unknown	15	816.9810048	s	15.6750080000000048	s	3.2353982580247553	V	11.776251237205134	Vs	-27.848210770280545	%
48	16	MX018-1	Unknown	16	861.08	s	15.6750079999999934	s	2.6420021702505909	V	10.178447921744036	Vs	-29.419307075899681	%
49	17	MX018-1	Unknown	17	1302.2790016	s	22.362995199999987	s	2.1091102591782533	V	40.090989043841918	Vs	-3.7	%
50	18	MX018-1	Unknown	18	1352.648	s	22.362995199999987	s	2.1115093188101324	V	40.2156331730146	Vs	-3.6927708634734158	%
51	19	MX018-1	Unknown	19	1402.3900032	s	22.5720064000000191	s	2.1109186532390716	V	40.248074004554738	Vs	-3.7440564811306309	%
52	1	MX018-1	Unknown	1	48.6969884	s	22.5719936000000003	s	2.1138592042654332	V	40.199061855058922	Vs	-3.5289433167441375	%
53	2	MX018-1	Unknown	2	98.4389888	s	22.5719936	s	2.1170667786609303	V	40.37664496735578	Vs	-3.649209189276803	%
54	3	MX018-1	Unknown	3	147.7629952	s	22.5720063999999992	s	2.1135404702107721	V	40.300890824428067	Vs	-3.7655472327445816	%
55	4	MX018-1	Unknown	4	198.1319936	s	22.3630080000000008	s	2.1144347484842396	V	40.344361680030715	Vs	-3.7873352972539465	%
56	5	MX018-1	Unknown	5	247.8739968	s	22.3629952	s	2.1128677645121581	V	40.277910714404513	Vs	-3.8090268593483634	%
57	6	MX018-1	Unknown	6	297.616	s	22.571993599999985	s	2.1142548593326969	V	40.303770739274405	Vs	-3.7948412564333678	%
58	7	MX018-1	Unknown	7	347.5669888	s	22.571993599999985	s	2.1134676425384349	V	40.296029016340359	Vs	-3.8301796449795689	%
59	8	MX018-1	Unknown	8	397.0999936	s	22.5720063999999964	s	2.1119434796693839	V	40.254678848890736	Vs	-3.8379130884776957	%
60	9	MX018-1	Unknown	9	447.0509952	s	22.5720063999999964	s	2.1105618066477895	V	40.217158449337695	Vs	-3.7	%
61	10	MX018-1	Unknown	10	667.9639936	s	13.7939968000000059	s	2.1931157544711368	V	5.5487623913287738	Vs	-28.189995244019329	%
62	11	MX018-1	Unknown	11	685.52	s	12.1219968000000034	s	3.546887793352146	V	8.60540497309292	Vs	-27.829329957168468	%
63	12	MX018-1	Unknown	12	706.8379904	s	8.9869952000000239	s	3.3913262566432097	V	8.43728787774864	Vs	-27.835846225450879	%
64	13	MX018-1	Unknown	13	710.6	s	5.6429951999999973	s	0.37360212016964783	V	0.90622342022057645	Vs	-29.747935822968973	%
65	14	MX018-1	Unknown	14	766.6119936	s	15.6750079999999934	s	3.197342742343893	V	10.234397955127406	Vs	-13.561224243801462	%
66	15	MX018-1	Unknown	15	816.1449984	s	15.2569983999999929	s	2.8370777548803292	V	9.7986703614597648	Vs	-27.69582789133651	%
67	16	MX018-1	Unknown	16	860.452992	s	16.0930047999999903	s	2.5138174228054013	V	8.9579352016910558	Vs	-29.4421533542083	%
68	17	MX018-1	Unknown	17	1302.6969884	s	22.3629952000000114	s	2.1089672293610406	V	40.13150372661714	Vs	-3.7	%
69	18	MX018-1	Unknown	18	1352.648	s	22.3629952000000114	s	2.1120488172951148	V	40.201507770522886	Vs	-3.68752005800721	%
70	19	MX018-1	Unknown	19	1402.3899904	s	22.3629952000000114	s	2.109628095086435	V	40.185949608094973	Vs	-3.8091551146243185	%

Data Report

Report content

- Report Settings
 - Image
 - Page
 - Page header
 - Page footer
- Content
 - Table: LabBook
 - Text: Sample List Title
 - Page Break: Space
 - Table: Sample List
 - Page Break: Page Break
 - Grouping: Loop through Sample List
 - Table: Sample line Data
 - Graph: Ratios
 - Graph: Main Chromatogram
 - Table: Peaks Data**
 - Page Break: Page Break

Common

Name: Peaks Data

Description: Table with basic Peaks Data and delta values

Use in Report

Columns Calculations Layout Bookmark

Source: Peaks Select Unique Values

Columns: Result columns: + x | ↑ ↓

Name	Common Caption	Repeat	Visible	Width	Merge Column	Separator	Format Column	Text	Calculations Use for label
Peak Number	Peak ID	<input type="checkbox"/>	<input checked="" type="checkbox"/>	auto	<None>		<None>		<input type="checkbox"/>
Compound Name	Compound Name	<input type="checkbox"/>	<input checked="" type="checkbox"/>	auto	<None>		<None>		<input type="checkbox"/>
Retention Time	Retention Time [s]	<input type="checkbox"/>	<input checked="" type="checkbox"/>	50.00 pt	<None>		<None>		<input type="checkbox"/>
Peak Width	Width [s]	<input type="checkbox"/>	<input checked="" type="checkbox"/>	50.00 pt	<None>		<None>		<input type="checkbox"/>
Peak Intensity 44.00 m/z	Intensity 44 m/z [V]	<input type="checkbox"/>	<input checked="" type="checkbox"/>	50.00 pt	<None>		<None>	f2	<input type="checkbox"/>
Peak Background 44.00 m/z	BGD 44 m/z [V]	<input type="checkbox"/>	<input type="checkbox"/>	50.00 pt	<None>		<None>	f3	<input type="checkbox"/>
Peak Area 44.00 m/z	Area 44 m/z [Vs]	<input type="checkbox"/>	<input checked="" type="checkbox"/>	50.00 pt	<None>		<None>	f3	<input type="checkbox"/>
d 13C/12C	δ13C [%]	<input type="checkbox"/>	<input checked="" type="checkbox"/>	50.00 pt	<None>		<None>	f2	<input type="checkbox"/>
d 13C/12C (ext. ref.)	δ13C [%] (Ext.Ref. Corr.)	<input type="checkbox"/>	<input checked="" type="checkbox"/>	50.00 pt	<None>		<None>	f2	<input type="checkbox"/>
d 18O/16O	δ18O [%]	<input type="checkbox"/>	<input type="checkbox"/>	50.00 pt	<None>		<None>	f2	<input type="checkbox"/>

Sorting | + x | ↑ ↓

Name	Sort Order	Name	Operator	Condition
Compound Name		Compound Name	is in list	Etio, Andros, 11-Keto, Testo, 11-OHE, 5β-diol, 5α-diol, PD, EpiT, 11-OHA
Label		Label	is in list	<input type="checkbox"/> Solvent <input type="checkbox"/> MX018-1 <input type="checkbox"/> MX018-2 <input type="checkbox"/> F1_QCN_11-Keto <input type="checkbox"/> F2_QCN_Testo <input type="checkbox"/> F2_QCN_11-EpiT

Data Report

GC Report
9/18/2023 12:24:32 PM



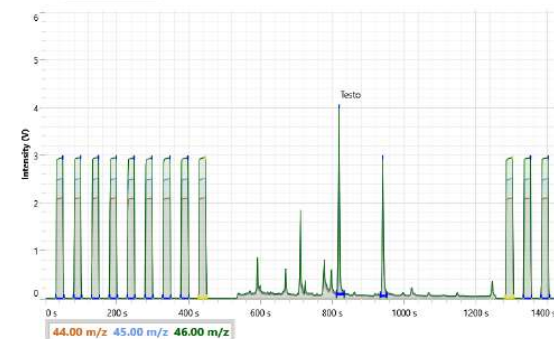
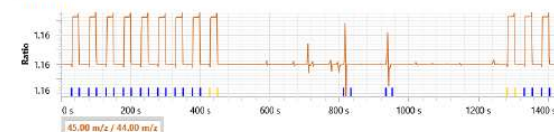
Sample List

Index	Label	Sample Type	Reference	Start Time	Comment
1	Solvent	Unknown		2023-02-01 06:26	
2	MX018-1	ChromReference	MX018-1	2023-02-01 06:54	5 ngul
3	MX018-1	Unknown		2023-02-01 07:22	5 ngul
4	MX018-1	Unknown		2023-02-01 07:50	5 ngul
5	MX018-1	Unknown		2023-02-01 08:18	5 ngul
6	MX018-2	Unknown		2023-02-01 08:46	5 ngul
7	MX018-2	Unknown		2023-02-01 09:14	5 ngul
8	MX018-2	Unknown		2023-02-01 09:42	5 ngul
9	Solvent	Unknown		2023-02-01 10:10	
10	Solvent	Unknown		2023-02-01 10:41	
11	F1_QCN_11-Keto	Unknown		2023-02-01 11:09	
12	F2_QCN_Testo	Unknown		2023-02-01 11:37	
13	F3_QCN_11-EpiT	Unknown		2023-02-01 12:05	
14	F4_QCN_5b-diol	Unknown		2023-02-01 12:33	
15	F5_QCN_5a-diol	Unknown		2023-02-01 13:01	
16	F6_QCN_PD	Unknown		2023-02-01 13:29	
17	MX018-1	Unknown		2023-02-01 13:57	5 ngul
18	MX018-2	Unknown		2023-02-01 14:25	5 ngul
19	F1_QCP_11-Keto	Unknown		2023-02-01 14:53	
20	F2_QCP_Testo	Unknown		2023-02-01 15:21	
21	F3_QCP_11-EpiT	Unknown		2023-02-01 15:49	
22	F4_QCP_5b-diol	Unknown		2023-02-01 16:17	
23	F5_QCP_5a-diol	Unknown		2023-02-01 16:45	
24	F6_QCP_PD	Unknown		2023-02-01 17:13	
25	MX018-1	Unknown		2023-02-01 17:41	5 ngul
26	MX018-2	Unknown		2023-02-01 18:09	5 ngul

GC Report
9/18/2023 12:24:32 PM



LabBook Steroids_13C_PTV_LVI_DB35MS_AuxGas inGC - Sintered liner - 25ul - 20230201 - KCL - B01 - GCs.imexp
 Sample Index 12
 Label F2_QCN_Testo
 Sample Type Unknown
 Start Time 2023-02-01 11:37:54
 Comment



Peak ID	Compound Name	Retention Time [s]	Width [s]	Intensity 44 m/z [V]	Area 44 m/z [Vs]	δ13C [‰]	δ13C [‰] (Ext. Ref. Corr.)
15	Testo	13:38	21.53	2.86	10.647	-24.32	-24.36

Data Integrity / Access Control

Key elements:

- **Audit Trails** for traceability of all actions
- **Access authorization** for system operation and results generation
- **Checks and controls** for analytical procedures
- **Secure retention and retrieval of records**
- **Electronic signatures** for full control of data generation, review and approval

Data Integrity / Access rights

The screenshot displays the 'Access Rights' configuration window in the ThermoFisher software. It is divided into two main sections: 'Application Access Rights' and 'Configurator Access Rights'. Both sections feature tables with columns for 'Application Name' or 'Configurator Name' and 'USER GROUPS' (System Administrator, Administrator, Data Administrator, Manager, Supervisor, Analyst, User). The status of each right is indicated by color-coded text: Allowed (green), Prohibited (red), and Prohibited (grey).

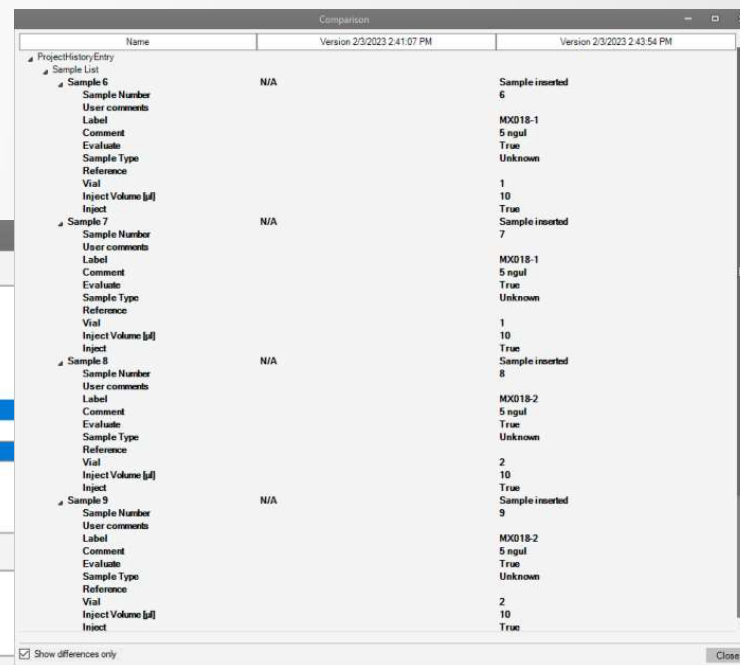
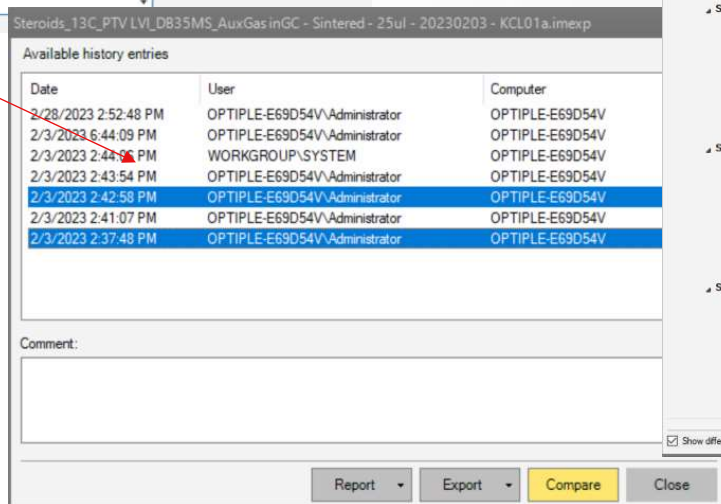
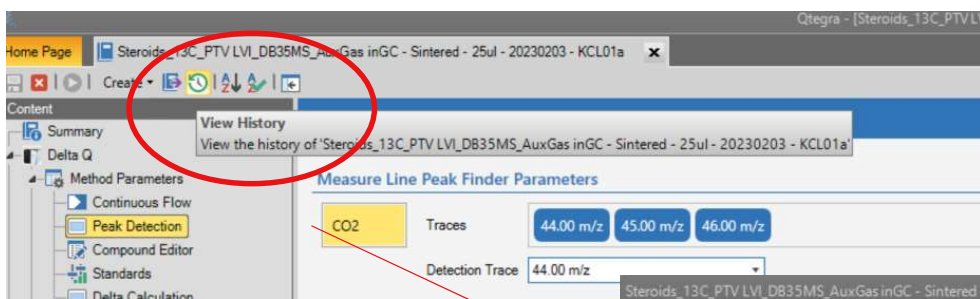
An 'Access Rights History' window is also visible, showing a list of entries with columns for Date, User, and Computer. The entries are as follows:

Date	User	Computer
2/16/2023 12:02:00	DESKTOP-2VG5558	DESKTOP-2VG5558
2/16/2023 12:01:95	DESKTOP-2VG5558	DESKTOP-2VG5558

At the bottom of the main window, there is a 'Comment' field containing 'Access Rights saved' and buttons for 'Export', 'Compare', and 'Close'. A 'Comparison' dialog box is also open, showing a tree view of permissions with 'Data Administrator' highlighted, and a table comparing 'Allowed' and 'Prohibited' states.

View history

LabBook changes history login



Digital Signature



Signature Workflow

Available signature workflow items

Display Name	Acquired By: Maria de Castro
Signing locks the LabBook	<input checked="" type="checkbox"/>

Display Name	Verified By:
Signing locks the LabBook	<input type="checkbox"/>

Display Name	Approved By:
Signing locks the LabBook	<input type="checkbox"/>

Instruments compatible with Qtegra ISDS Software

Thermo Scientific™

DELTA™ series IRMS:

- DELTA Q IRMS
- DELTA V Plus IRMS
- DELTA V Advantage IRMS

253 Plus™ 10 kV IRMS and MAT 253 IRMS

ConFlo IV™ Universal Interface

TRACE™ 1310 GC and GC IsoLink™ II Conversion Interface with:

- TriPlus™ RSH Autosampler
- or
- AI/AS 1310 Autosampler

GC-MS-IRMS Hyphenated System with Thermo Scientific™
ISQ 7000 with GC IsoLink II Conversion Interface

Thank you

