Thermo Fisher Scientific Software Update

María de Castro

GasIRMS Field Applications Specialist EMEA/Global

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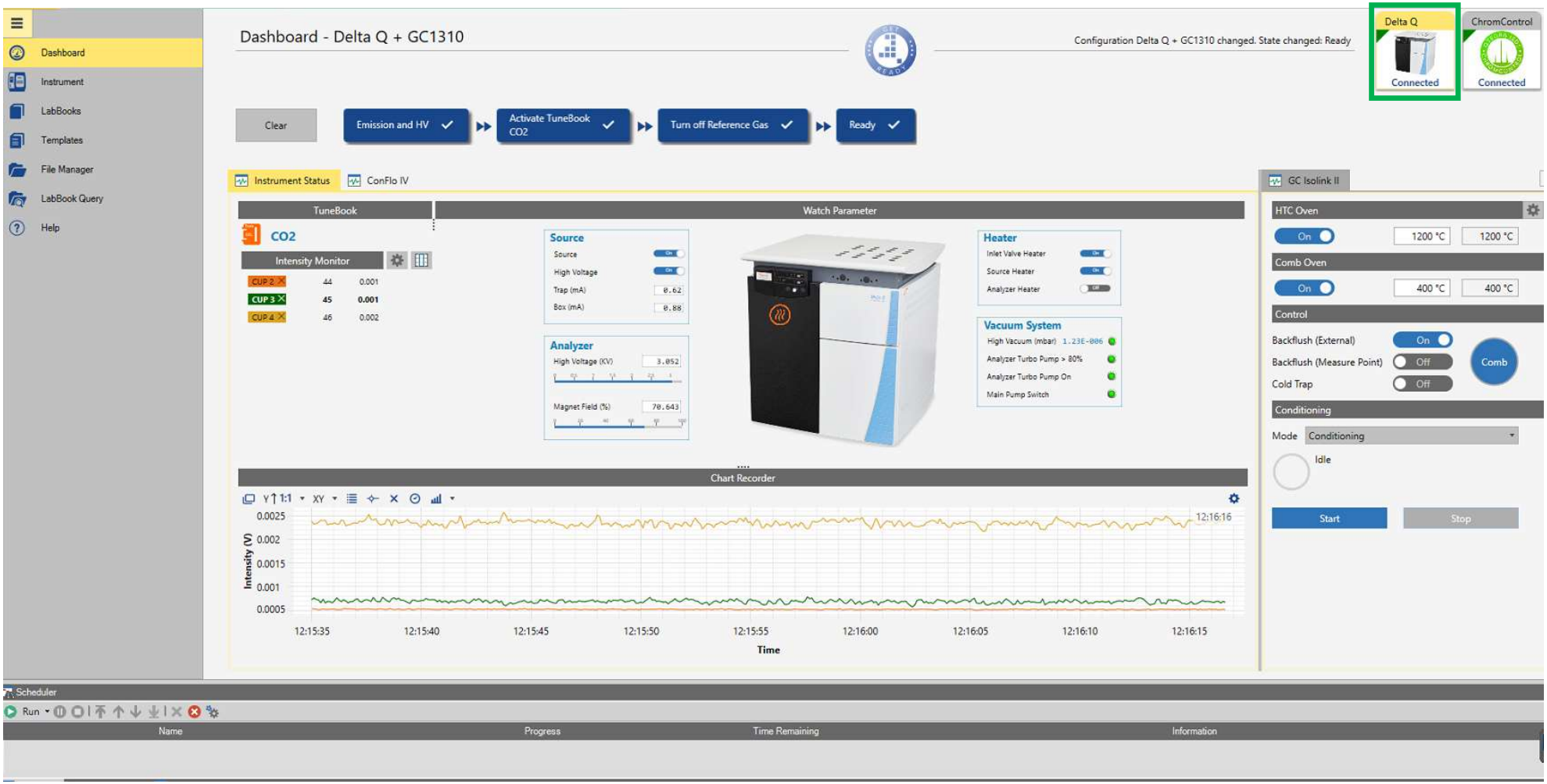
The world leader in serving science

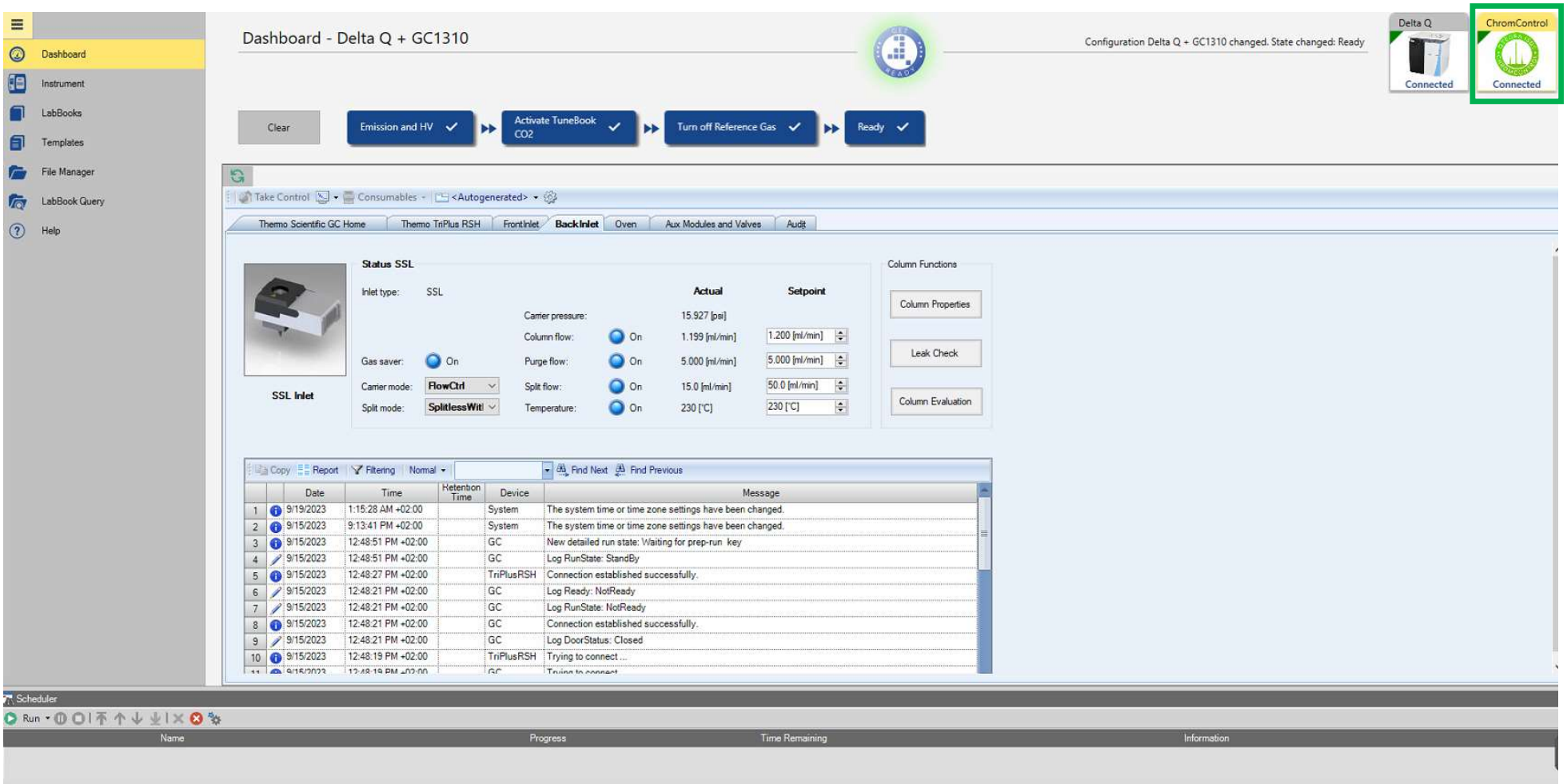
Software Releases

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

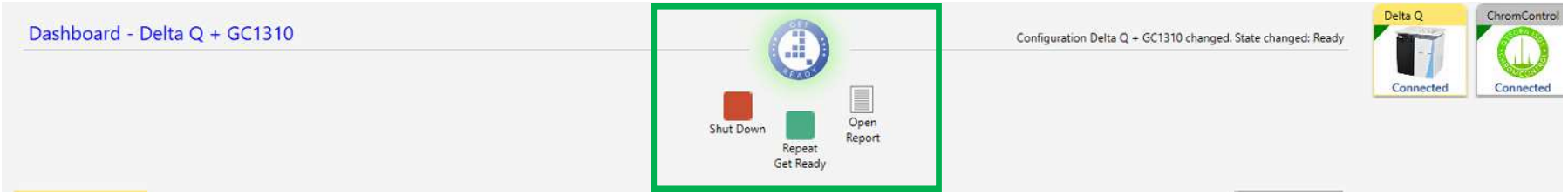
Dashboard

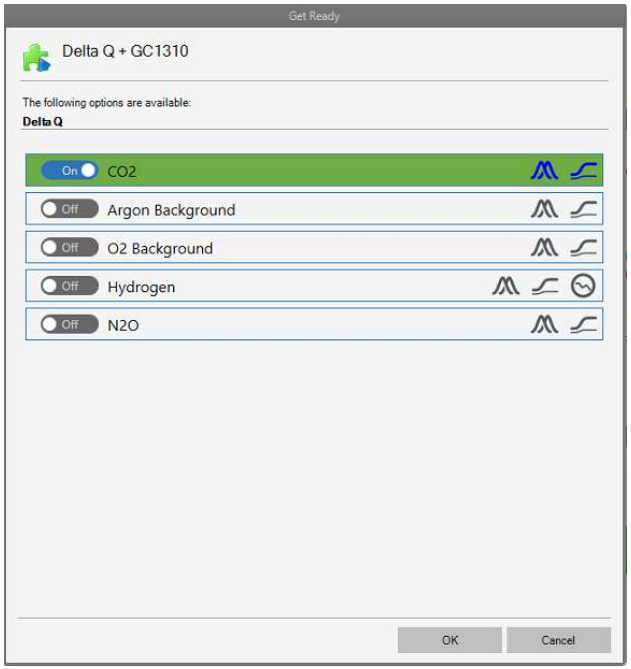

Dashboard
Instrument
LabBooks
Templates
File Manager
LabBook Query
Help
Dashboard - Delta Q + GC1310
Configuration Delta Q + GC1310 changed. State changed: Ready
Delta Q
Connected
ChromControl
Connected
Clear
Emission and HV
Activate TuneBook CO2
Turn off Reference Gas
Ready
Instrument Status
ConFlo IV
TuneBook
CO2
Intensity Monitor
CUP 2 44 0.001
CUP 3 45 0.001
CUP 4 46 0.002
Watch Parameter
Source
Source
High Voltage
Trap (mA) 0.62
Box (mA) 0.88
Analyzer
High Voltage (KV) 3.052
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)
0.0025
0.002
0.0015
0.001
0.0005
12:16:16
12:15:35
12:15:40
12:15:45
12:15:50
12:15:55
12:16:00
12:16:05
12:16:10
12:16:15
Time
GC Isolink II
HTC Oven
On
1200 °C
1200 °C
Comb Oven
On
400 °C
400 °C
Control
Backflush (External) On
Backflush (Measure Point) Off
Cold Trap Off
Comb
Conditioning
Mode Conditioning
Idle
Start
Stop
Scheduler
Run
Name
Progress
Time Remaining
Information

Dashboard

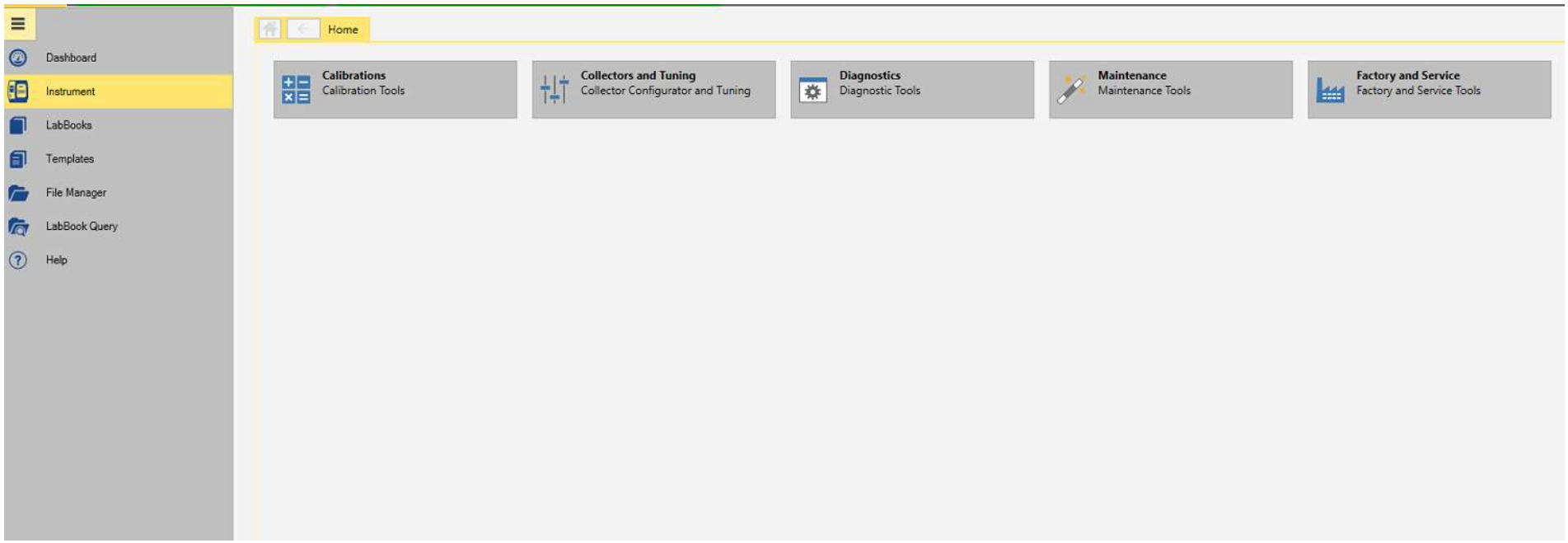

Dashboard
Instrument
LabBooks
Templates
File Manager
LabBook Query
Help
Dashboard - Delta Q + GC1310
Configuration Delta Q + GC1310 changed. State changed: Ready
Delta Q
Connected
ChromControl
Connected
Clear
Emission and HV
Activate TuneBook CO2
Turn off Reference Gas
Ready
Take Control
Consumables
<Autogenerated>
Thermo Scientific GC Home
Thermo TriPlus RSH
FrontInlet
BackInlet
Oven
Aux Modules and Valves
Audit
Status SSL
Inlet type: SSL
Actual
Setpoint
Carrier pressure: 15.927 [psi]
Column flow: On 1.199 [ml/min] 1.200 [ml/min]
Gas saver: On
Purge flow: On 5.000 [ml/min] 5.000 [ml/min]
Carrier mode: FlowCtrl
Split flow: On 15.0 [ml/min] 50.0 [ml/min]
Split mode: SplitlessWit
Temperature: On 230 [°C] 230 [°C]
SSL Inlet
Column Functions
Column Properties
Leak Check
Column Evaluation
Copy
Report
Filtering
Normal
Find Next
Find Previous
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 ...
Scheduler
Run
Name
Progress
Time Remaining
Information

Dashboard \ Get Ready

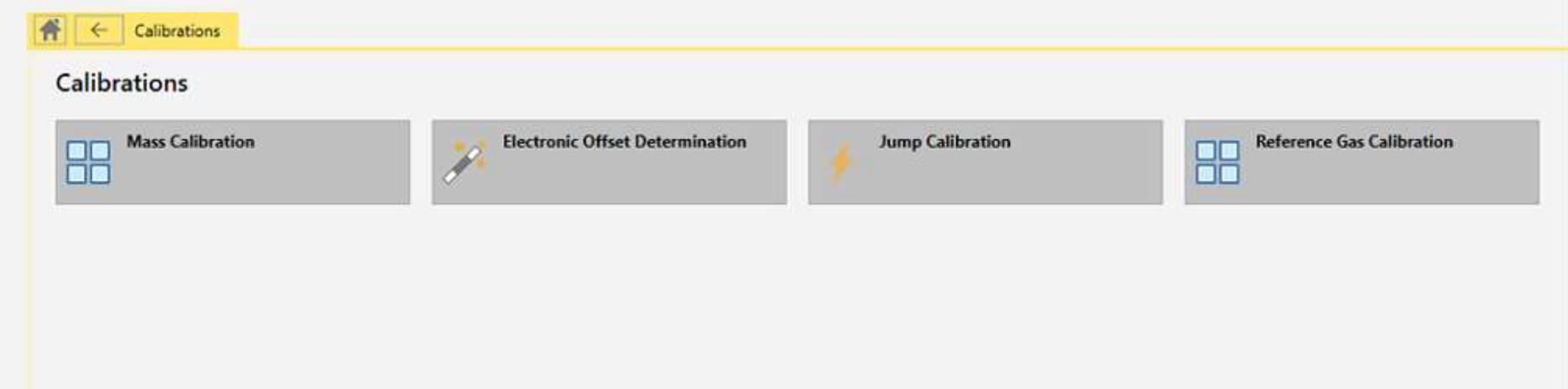




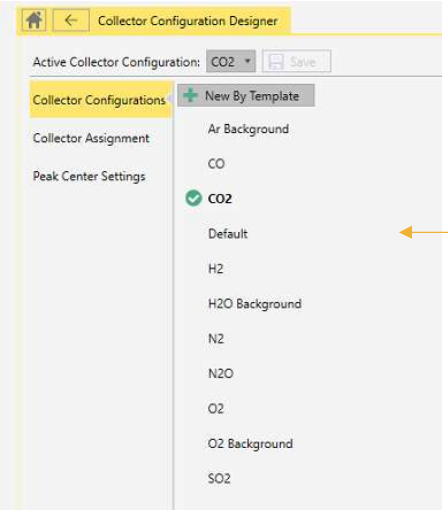
Instrument

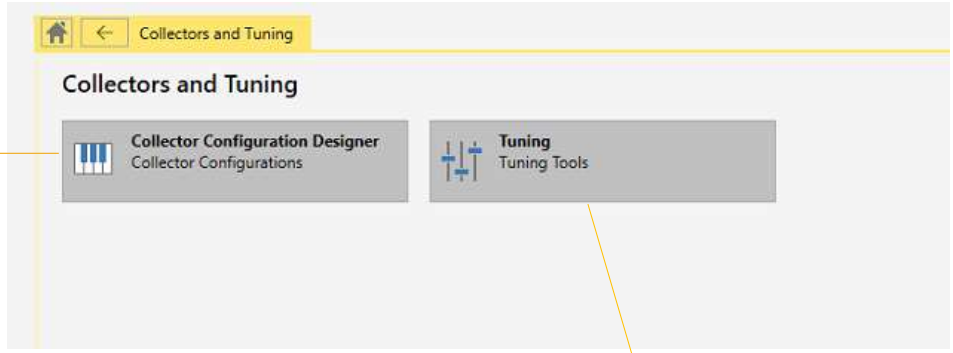

Dashboard
Instrument
LabBooks
Templates
File Manager
LabBook Query
Help
Home
Calibrations
Calibration Tools
Collectors and Tuning
Collector Configurator and Tuning
Diagnostics
Diagnostic Tools
Maintenance
Maintenance Tools
Factory and Service
Factory and Service Tools

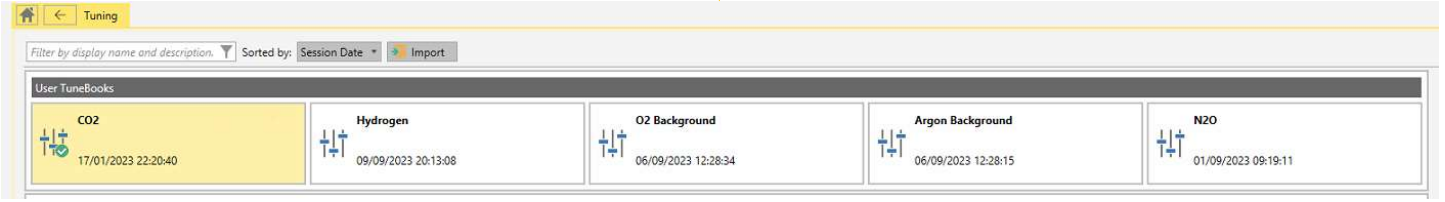
Instrument \ Calibrations



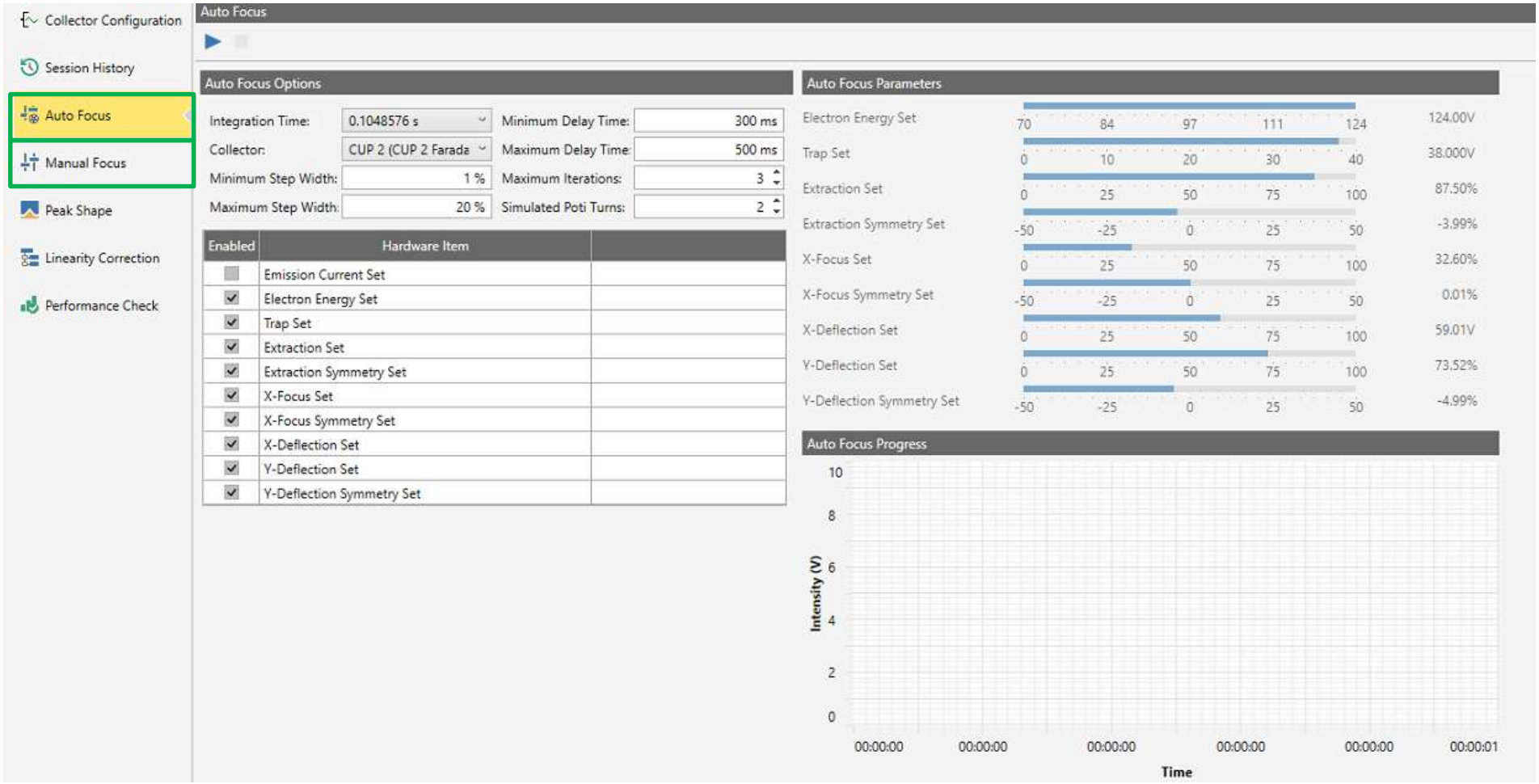
Instrument \ Collectors and Tuning



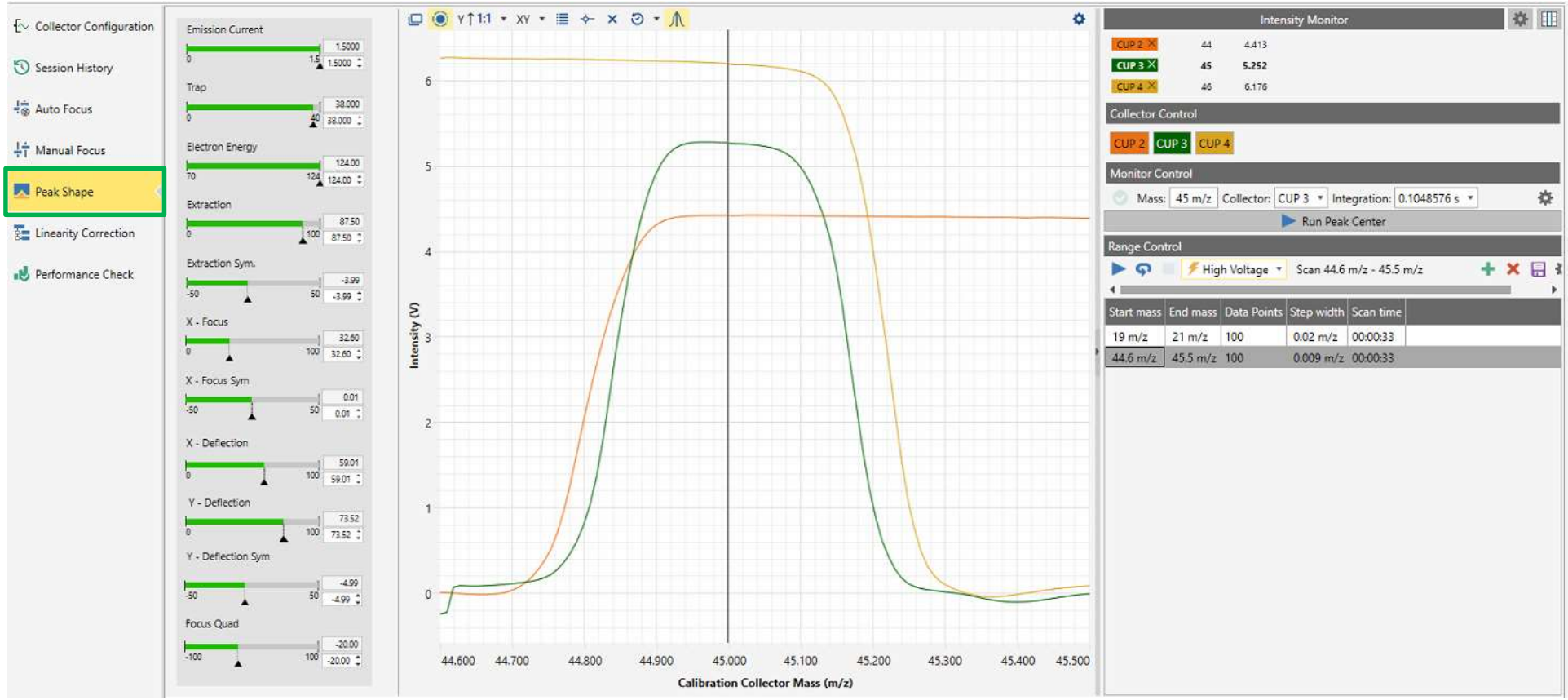




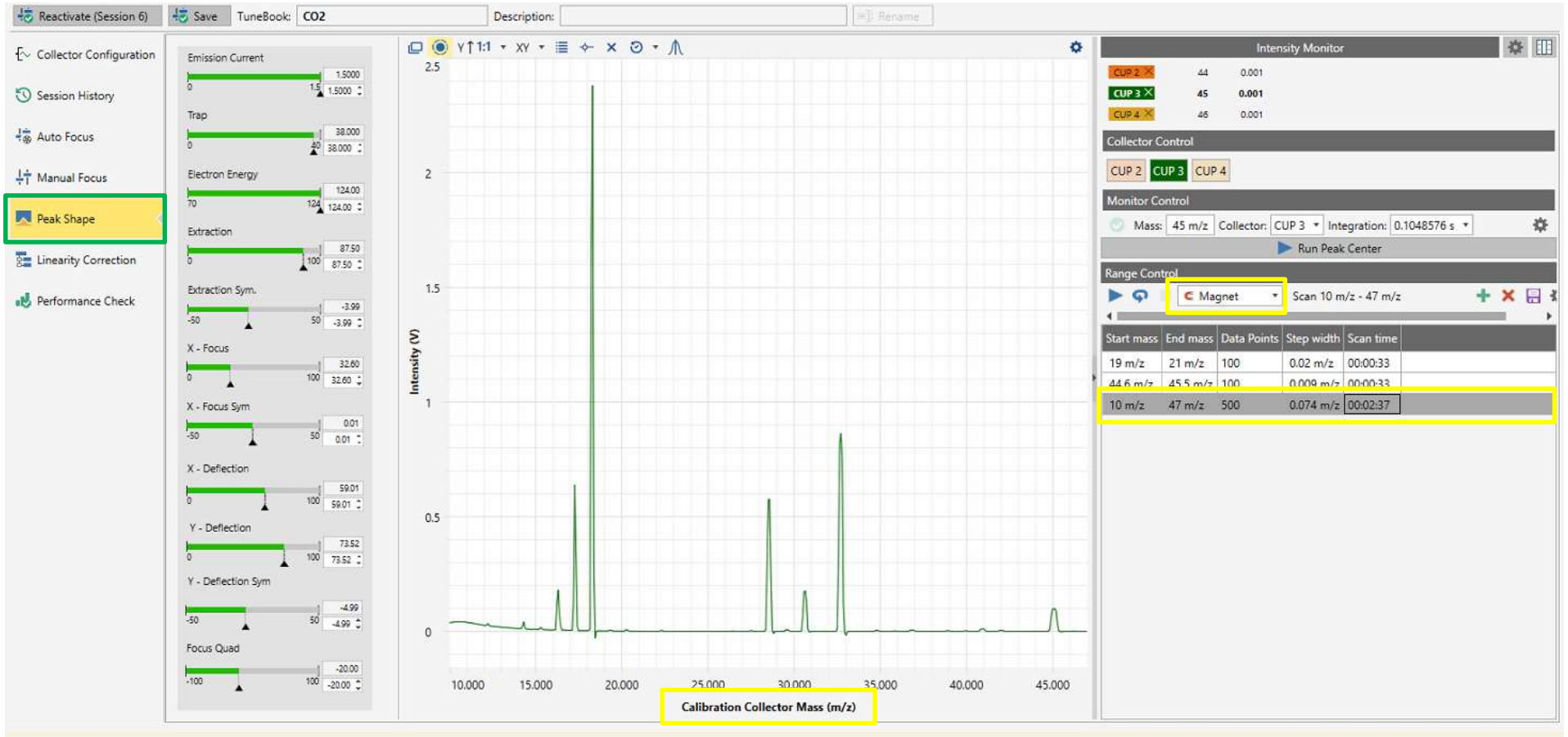
Instrument \ Collectors and Tuning \ Tunning \ CO_2



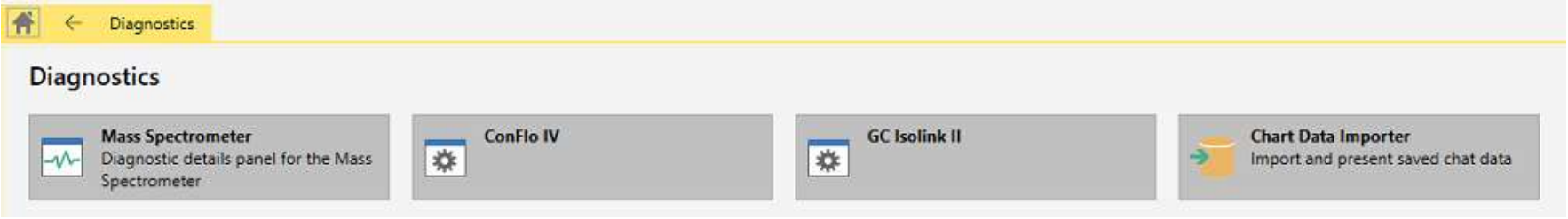
Instrument \ Collectors and Tuning \ Tunning \ CO_2



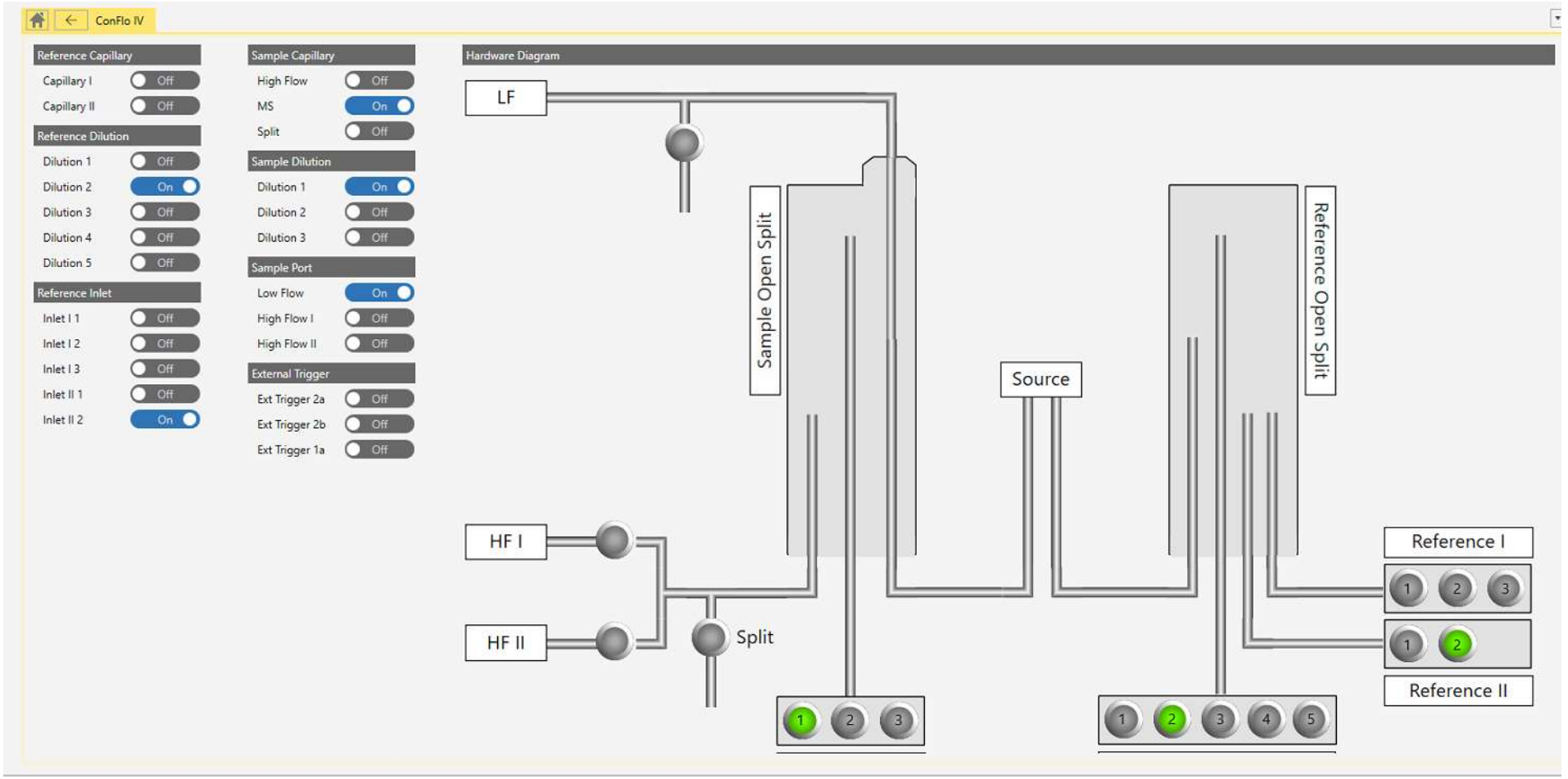
Instrument \ Collectors and Tuning \Tunning \ CO_2



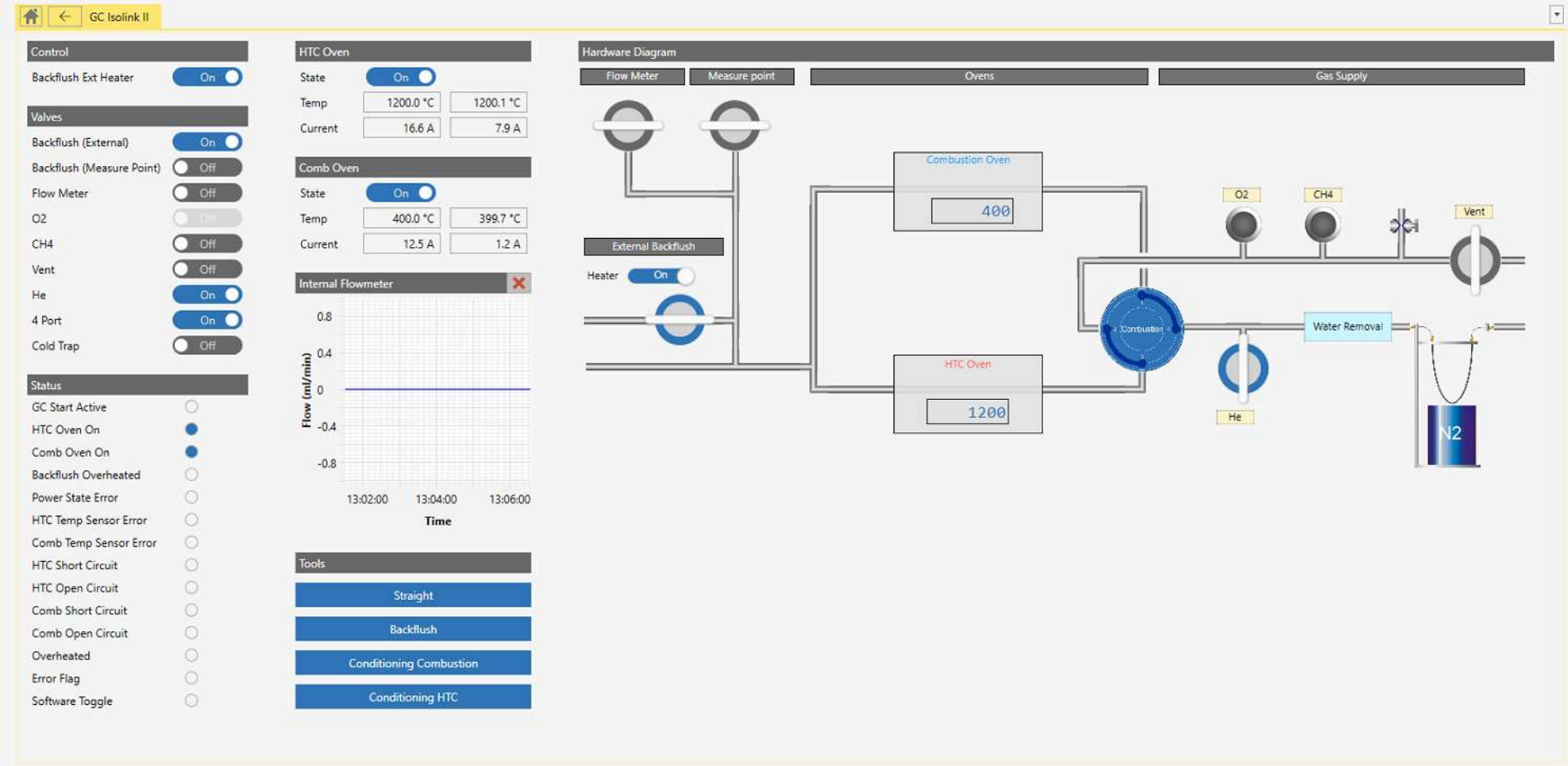
Instrument \ Diagnostics



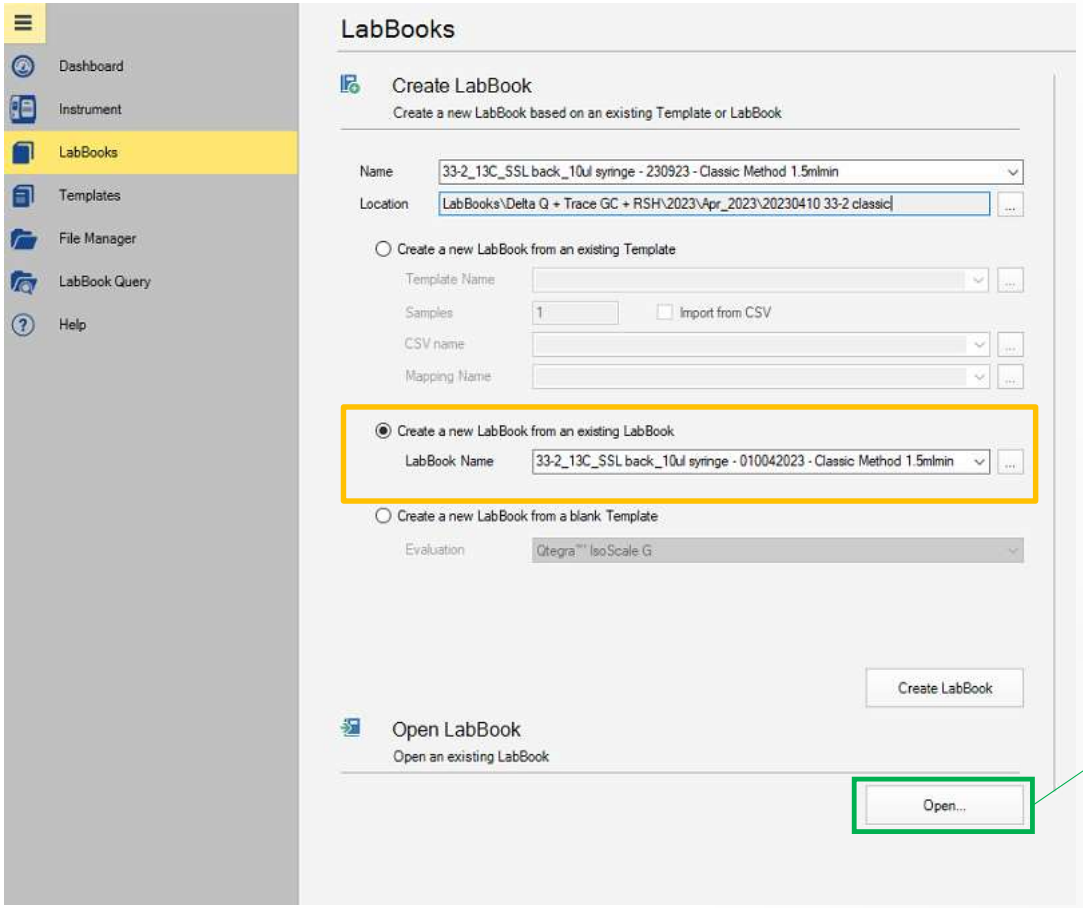
Instrument \ Diagnostics \ Conflo IV

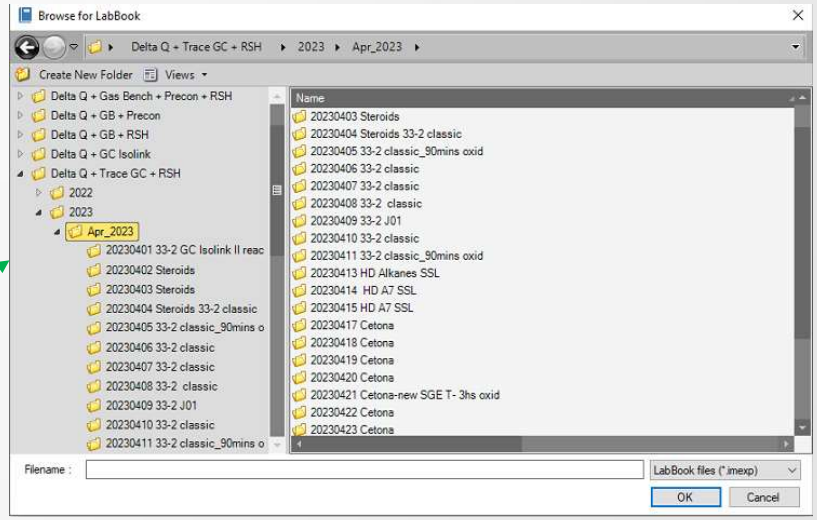


Instrument \ Diagnostics \ GC Isolink II

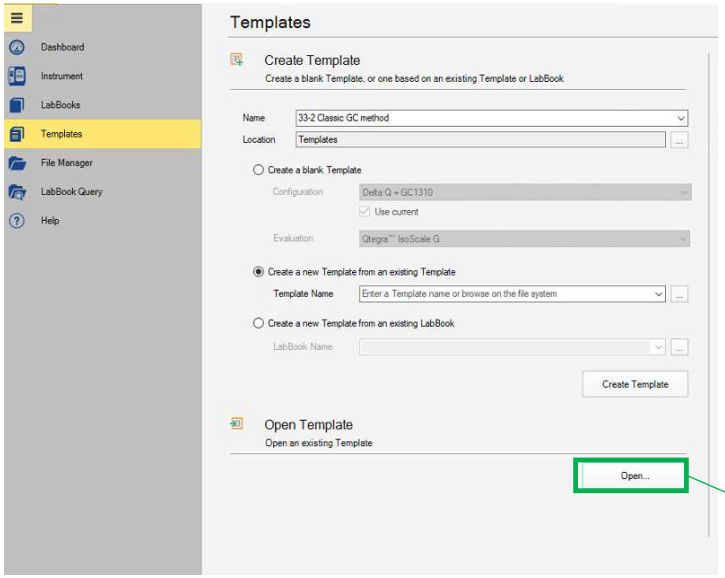


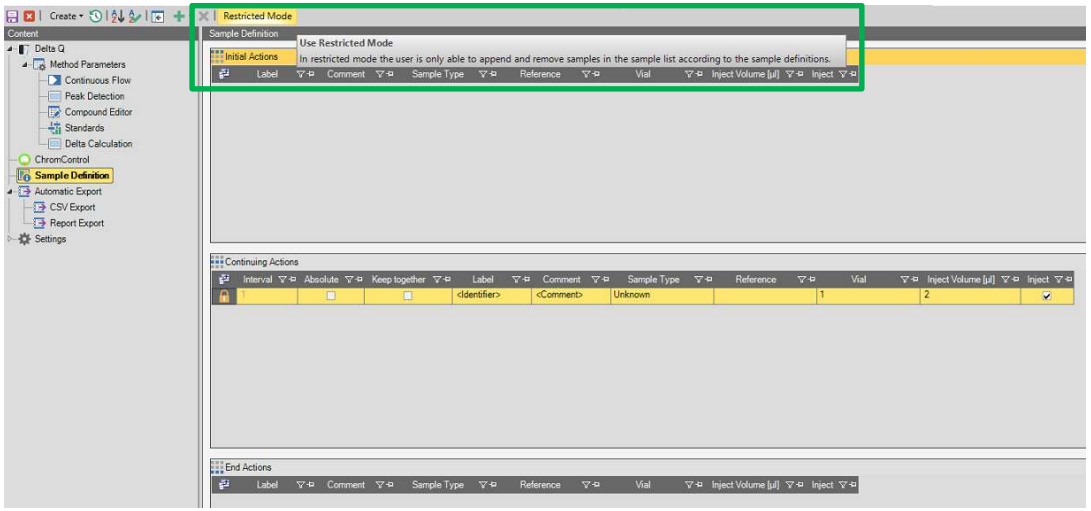
LabBooks

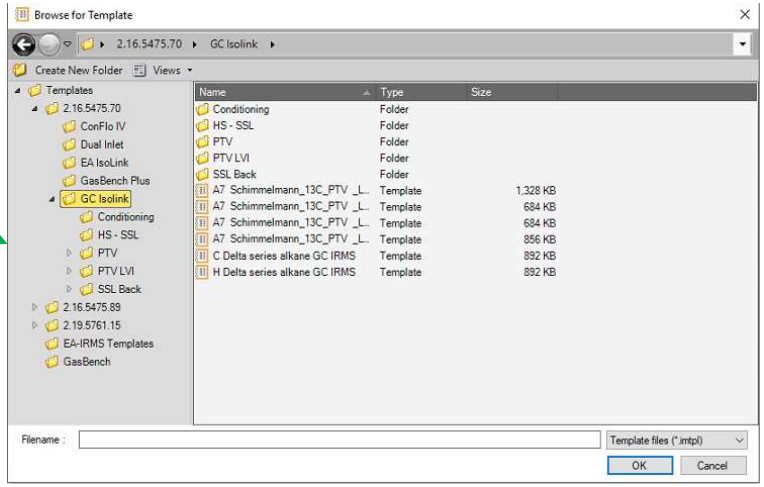

LabBooks
Dashboard
Instrument
LabBooks
Templates
File Manager
LabBook Query
Help
LabBooks
Create LabBook
Create a new LabBook based on an existing Template or LabBook
Name
33-2_13C_SSL back_10ul syringe - 230923 - Classic Method 1.5mlmin
Location
LabBooks\Delta Q + Trace GC + RSH\2023\Apr_2023\20230410 33-2 classic
Create a new LabBook from an existing Template
Template Name
Samples
1
Import from CSV
CSV name
Mapping Name
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 :
LabBook files (*.imexp)
OK
Cancel

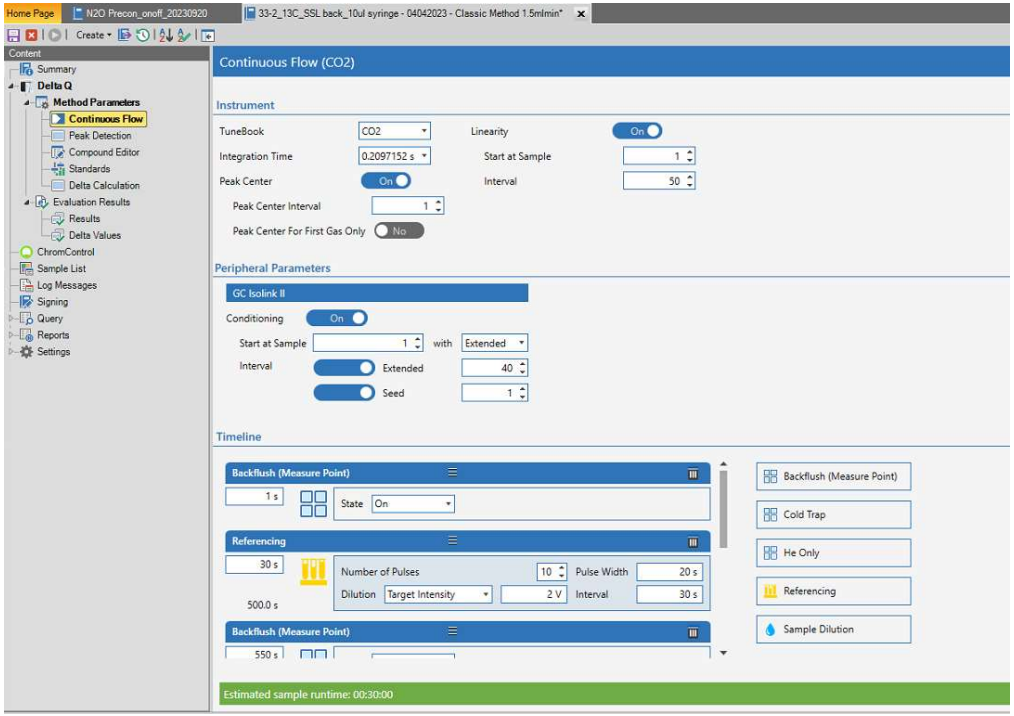
LabBookTemplates

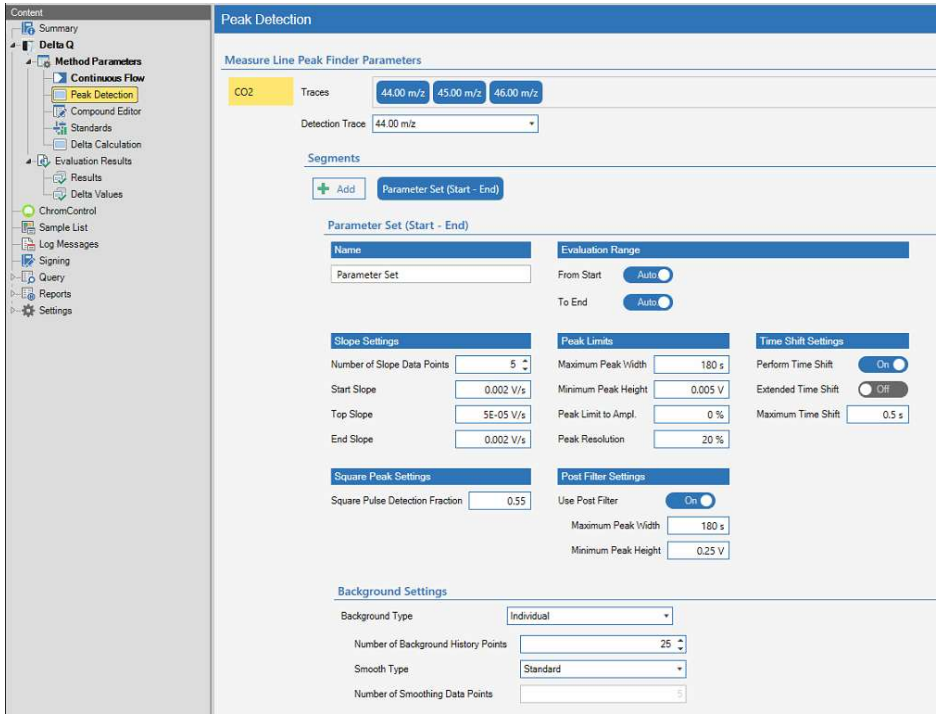




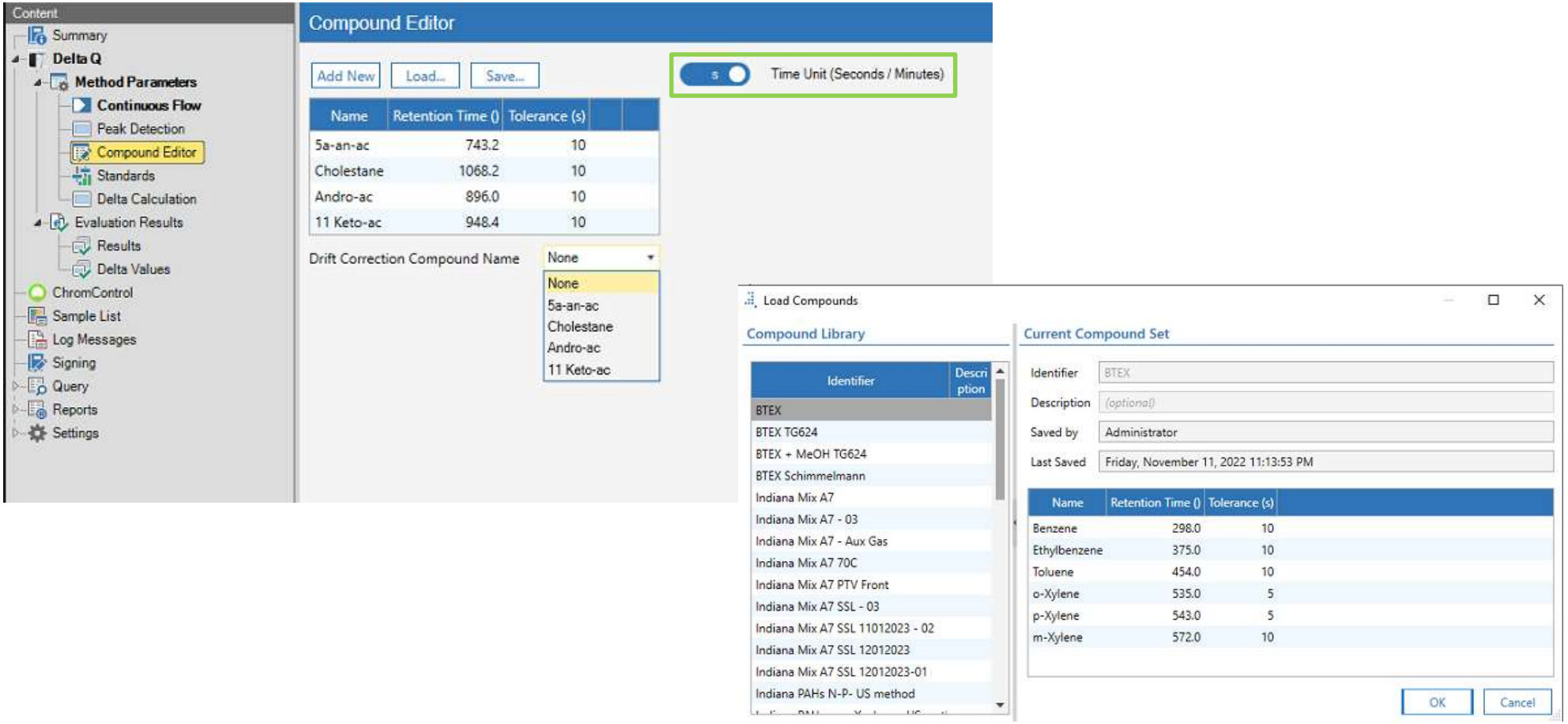


LabBook \ Continues Flow and Peak Detection

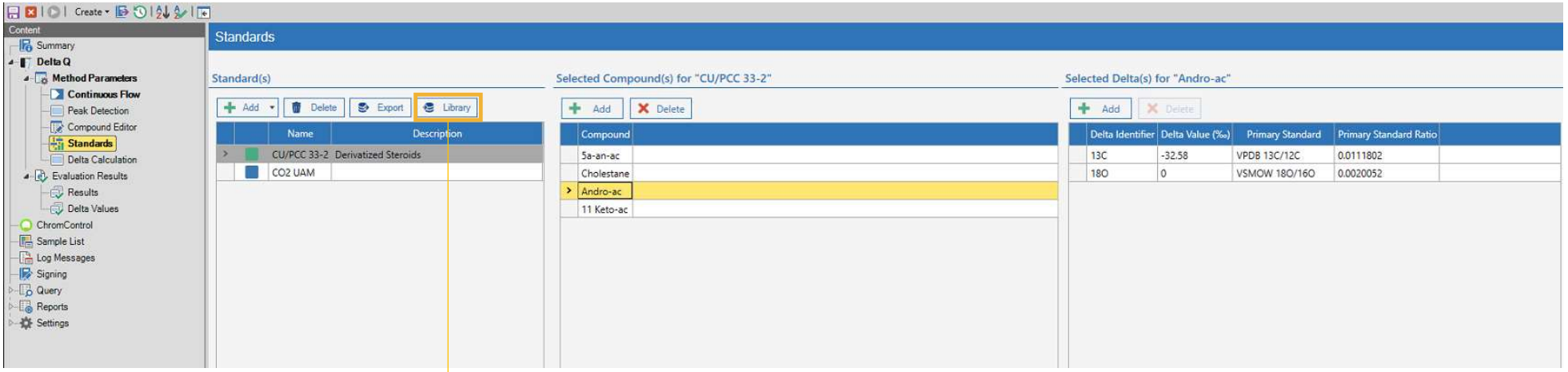


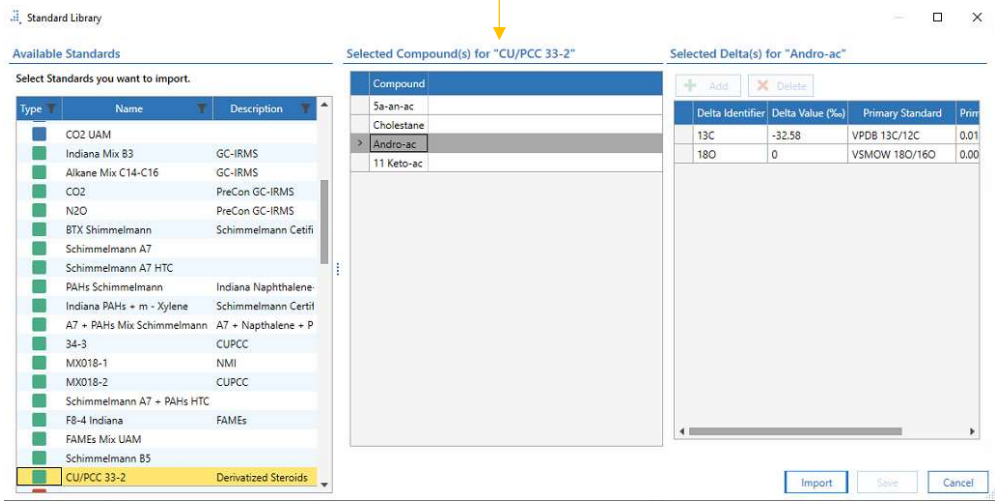


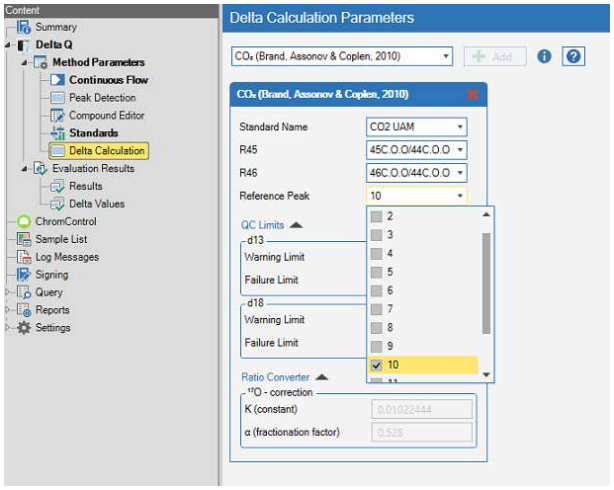
LabBook \ Compound Editor – Drift Correction



LabBook \ Standards and Delta Calculation Paremeters

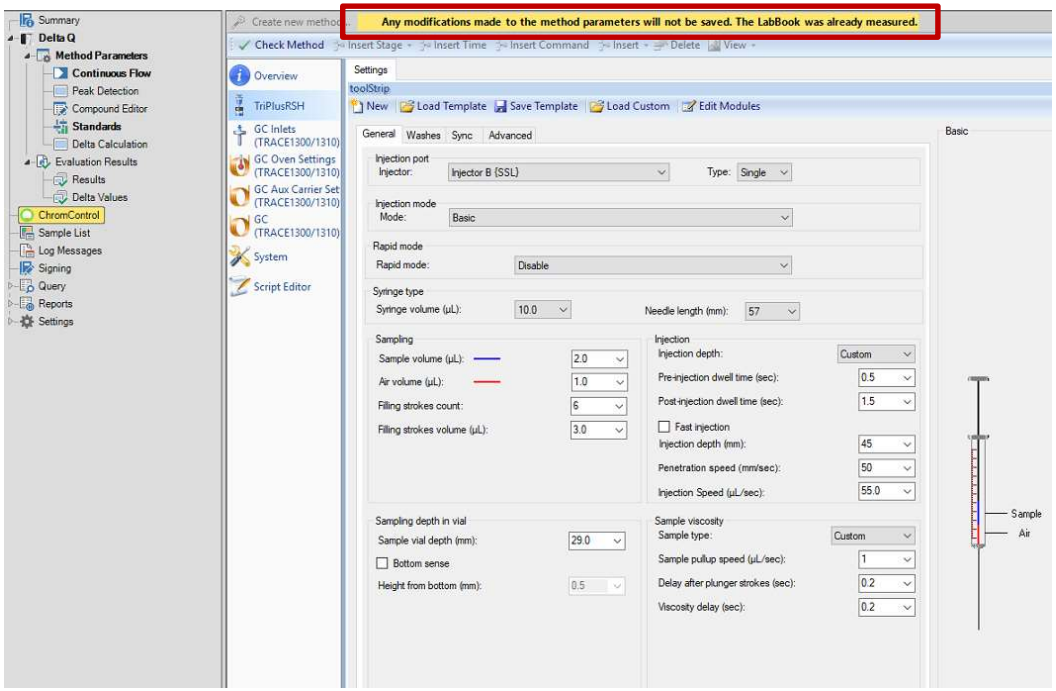


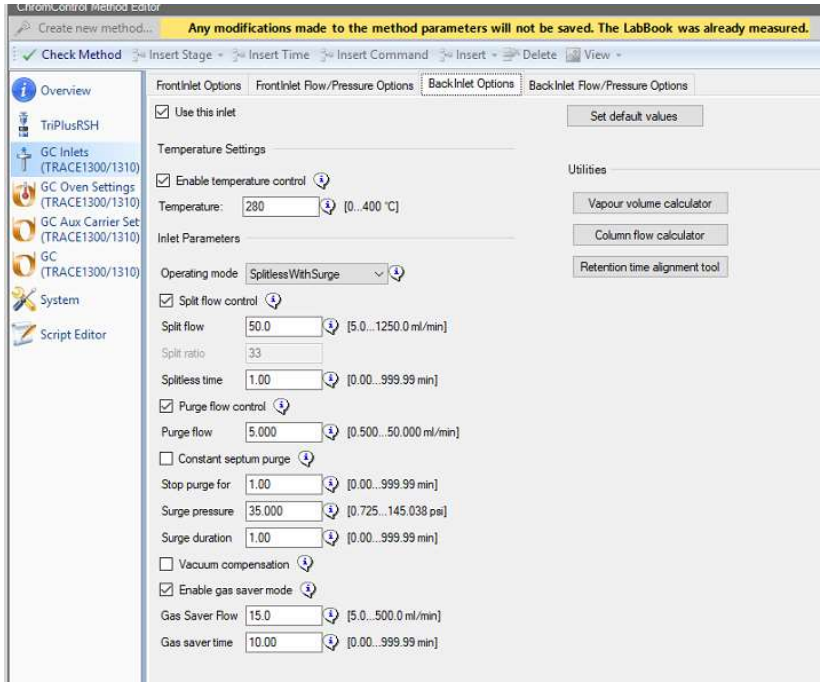




Autosampler and GC Methods: Chromcontrol

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





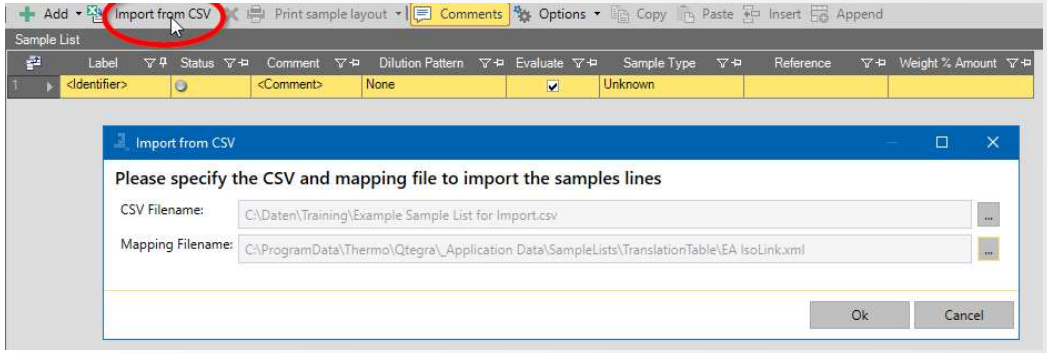
LabBook \ Sample List

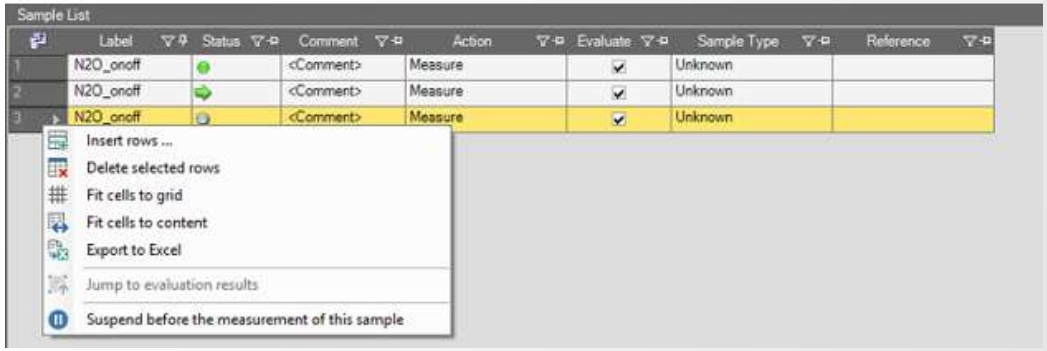
Sample List

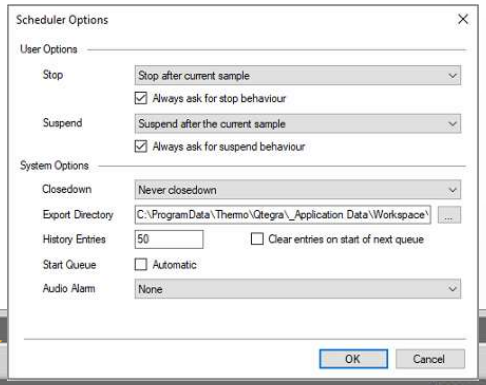
	Label	Status	Comment	Run ID	Evaluate	Sample Type	Reference	Vial	Inject Volume [µl]	Inject
1	Solvent			1	☑	Unknown		54	10	☑
2	MX018-1		5 ngul	2	☑	Delta Standard (CSIA)	MX018-1	20	10	☑
3	MX018-1		5 ngul	3	☑	Unknown		20	10	☑
4	MX018-1		5 ngul	4	☑	Unknown		20	10	☑
5	MX018-1		5 ngul	5	☑	Unknown		20	10	☑
6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

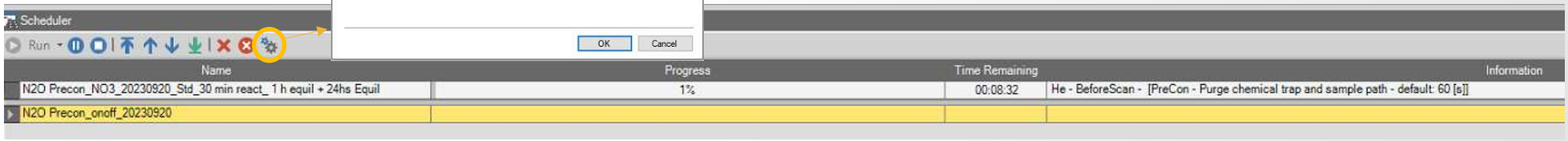
LabBook \ Sample List – Sequence Scheduler

- Import/Export Sample Lists (CSV)
- Ethe sample list when it´s alreay 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	☑			20	10	☑
5	MX018-1		5 ngul	5	☑			20	10	☑
6	MX018-2		5 ngul	6	☑			21	10	☑
7	MX018-2		5 ngul	7	☑			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	☑

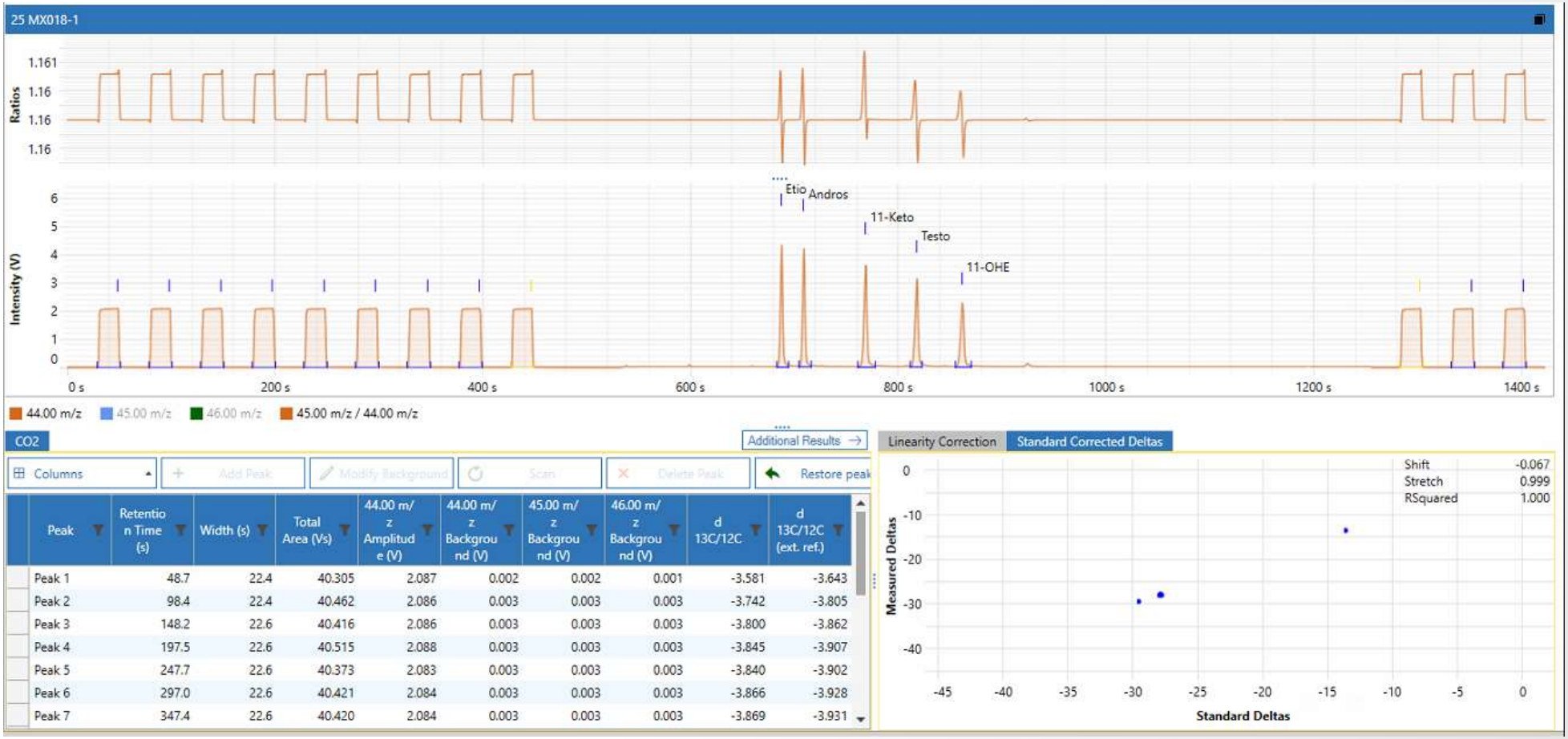
Conditioning
Delta Standard (CSIA)
Drift Correction
QC Standard
Ref Gas Calibration
Unknown

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	☑

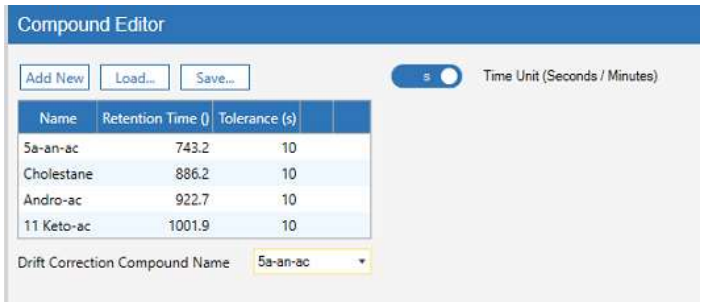
34-3
MX018-1
MX018-2

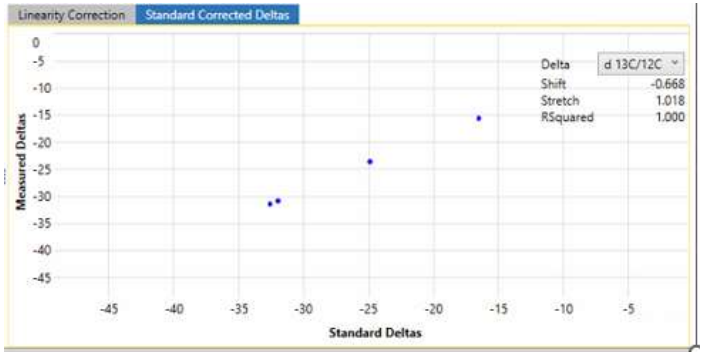
Data Normalization (External Referencing)



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.)
Peak 1	48.7	22.4	40.305	2.087	0.002	0.002	0.001	-3.581	-3.643
Peak 2	98.4	22.4	40.462	2.086	0.003	0.003	0.003	-3.742	-3.805
Peak 3	148.2	22.6	40.416	2.086	0.003	0.003	0.003	-3.800	-3.862
Peak 4	197.5	22.6	40.515	2.088	0.003	0.003	0.003	-3.845	-3.907
Peak 5	247.7	22.6	40.373	2.083	0.003	0.003	0.003	-3.840	-3.902
Peak 6	297.0	22.6	40.421	2.084	0.003	0.003	0.003	-3.866	-3.928
Peak 7	347.4	22.6	40.420	2.084	0.003	0.003	0.003	-3.869	-3.931

Drift Correction (Time correction)



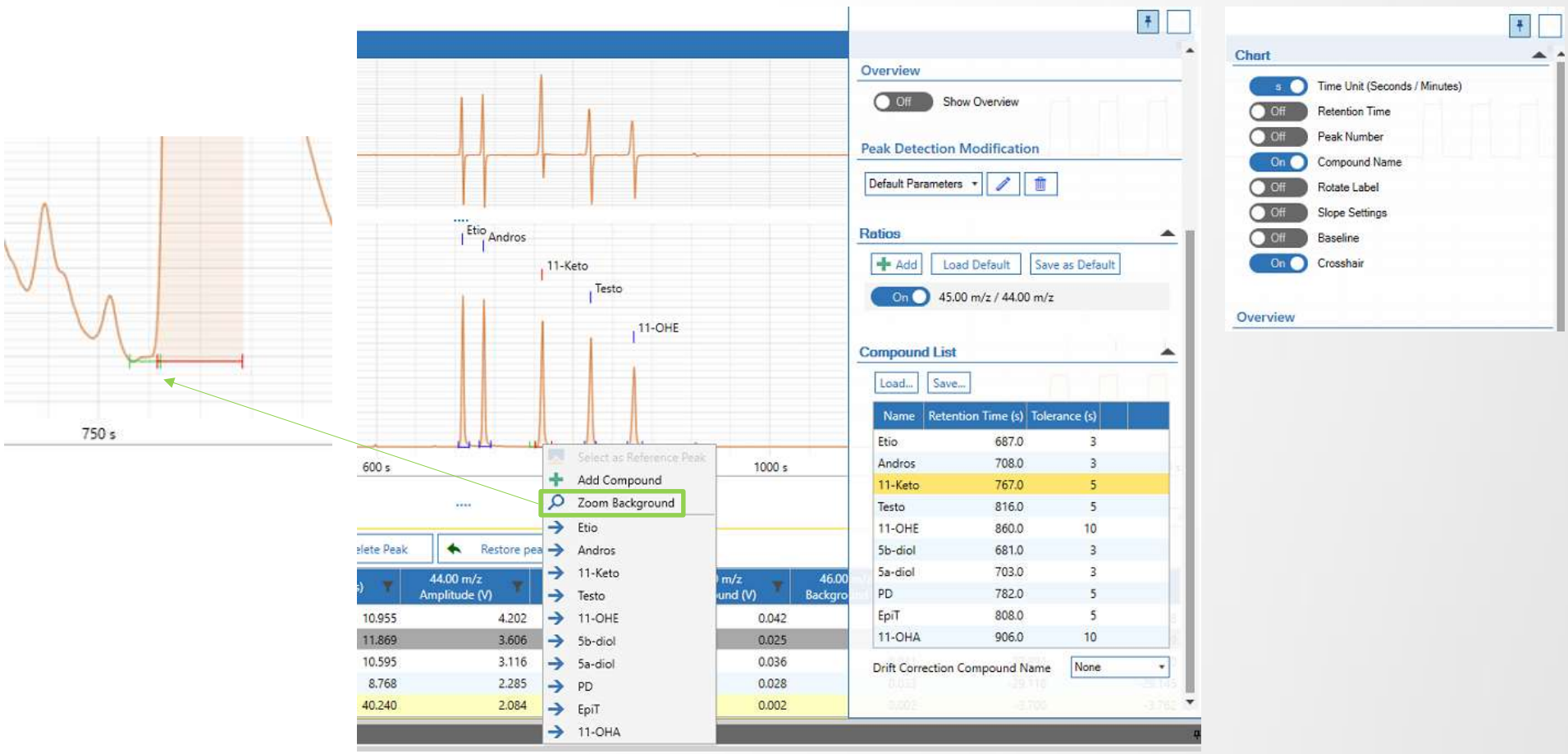


Sample List

	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	651.0	24.0	45.337	2.234	0.034	0.039	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 overlayed chromatogram view = better insight for method development

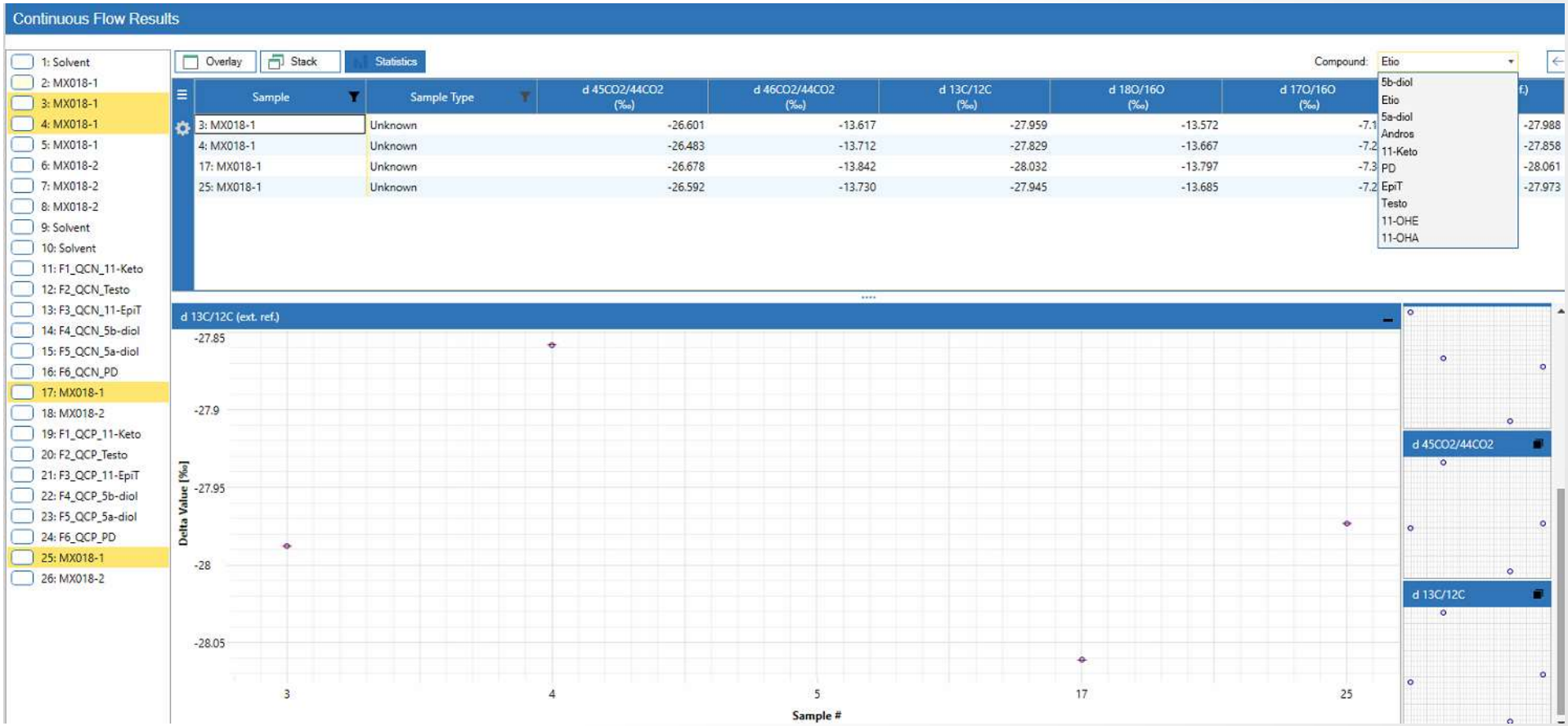
Data Visualization

Sample	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.)
16: F6_QCN_PD	(10) PD	783.8	14.0	17.759	5.287	0.023	0.026	0.030	-23.898	-23.932
24: F6_QCP_PD	(10) PD	781.2	10.2	2.854	0.999	0.021	0.025	0.028	-23.617	-23.652

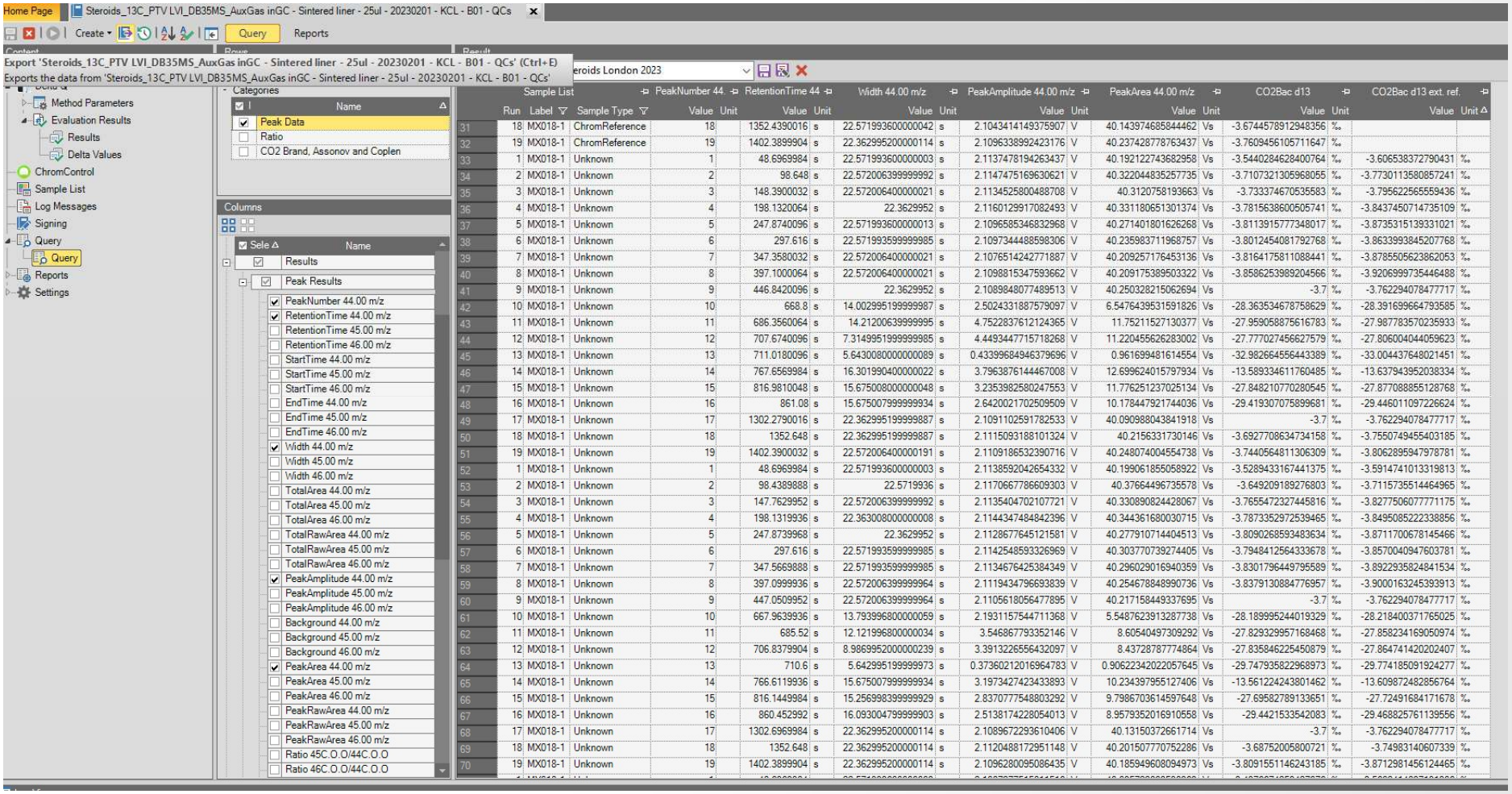
Data Visualization

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.)
(15) Testo	817.0	15.7	11.962	3.235	0.034	0.040	0.046	-27.848	-27.877
(15) Testo	816.1	15.3	9.953	2.837	0.033	0.039	0.045	-27.696	-27.725
(13) Testo	818.2	10.9	8.777	2.625	0.032	0.037	0.043	-27.752	-27.781
(13) Testo	818.0	11.3	10.595	3.116	0.031	0.036	0.041	-27.891	-27.920

Data Visualization

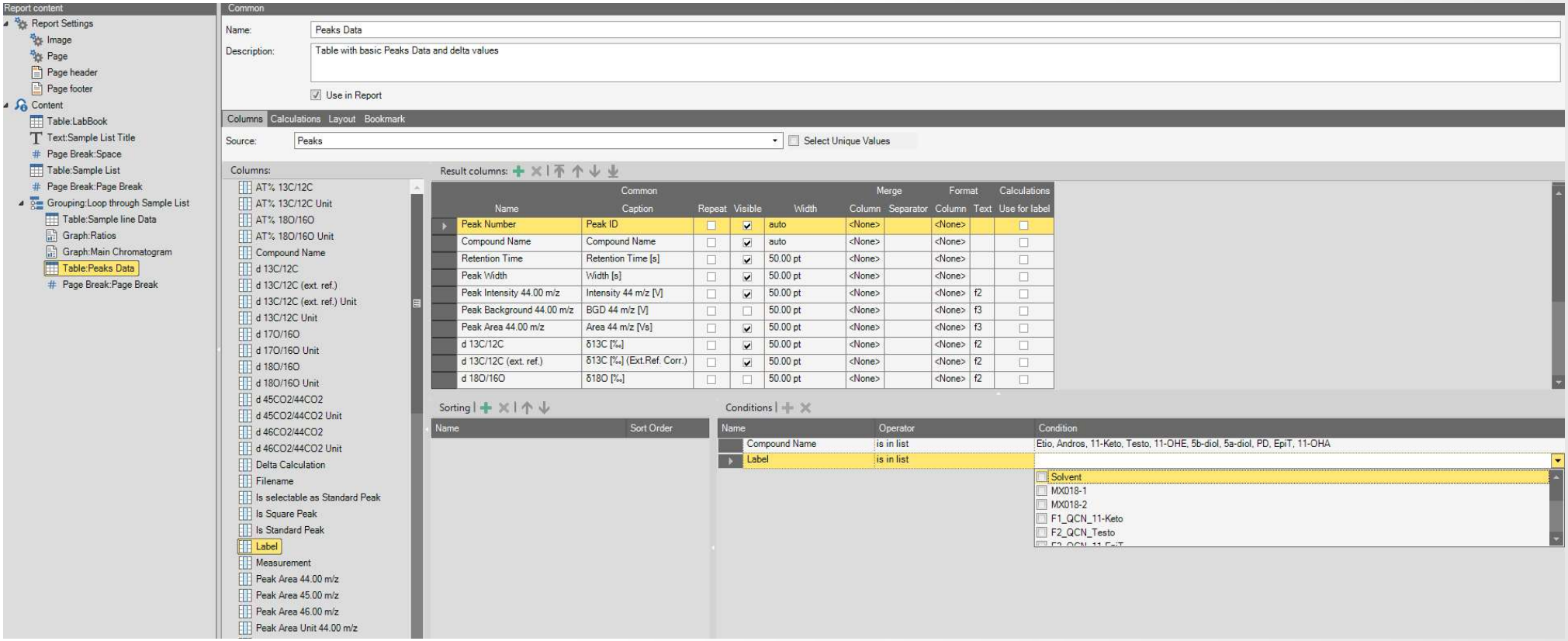


Data Export



	Sample List		PeakNumber 44.		RetentionTime 44		Width 44.00 m/z		PeakAmplitude 44.00 m/z		PeakArea 44.00 m/z		CO2Bac d13		CO2Bac d13 ext. ref.	
	Run	Label	Sample Type	Value	Unit	Value	Unit	Value	Unit	Value	Unit	Value	Unit	Value	Unit	Value	Unit
31	18	MX018-1	ChromReference	18		1352.4390016	s	22.571993600000042	s	2.1043414149375907	V	40.143974685844462	Vs	-3.6744578912948356	‰		
32	19	MX018-1	ChromReference	19		1402.3899904	s	22.362995200000114	s	2.1096338992423176	V	40.237428778763437	Vs	-3.7609456105711647	‰		
33	1	MX018-1	Unknown	1		48.6969984	s	22.571993600000003	s	2.1137478194263437	V	40.192122743682958	Vs	-3.5440284628400764	‰	-3.606538372790431	‰
34	2	MX018-1	Unknown	2		98.648	s	22.572006399999992	s	2.1147475169630621	V	40.322044835257735	Vs	-3.7107321305968055	‰	-3.7730113580857241	‰
35	3	MX018-1	Unknown	3		148.3900032	s	22.572006400000021	s	2.1134525800488708	V	40.3120758193663	Vs	-3.733374670535583	‰	-3.795622565559436	‰
36	4	MX018-1	Unknown	4		198.1320064	s	22.3629952	s	2.1160129917082493	V	40.331180651301374	Vs	-3.7815638600505741	‰	-3.8437450714735109	‰
37	5	MX018-1	Unknown	5		247.8740096	s	22.571993600000013	s	2.1096585346832968	V	40.271401801626268	Vs	-3.8113915777348017	‰	-3.8735315139331021	‰
38	6	MX018-1	Unknown	6		297.616	s	22.571993599999985	s	2.1097344488598306	V	40.235983711968757	Vs	-3.8012454081792768	‰	-3.8633993845207768	‰
39	7	MX018-1	Unknown	7		347.3580032	s	22.572006400000021	s	2.1076514242771887	V	40.209257176453136	Vs	-3.8164175811088441	‰	-3.8785505623862053	‰
40	8	MX018-1	Unknown	8		397.1000064	s	22.572006400000021	s	2.1098815347593662	V	40.209175389503322	Vs	-3.8586253989204566	‰	-3.9206999735446488	‰
41	9	MX018-1	Unknown	9		446.8420096	s	22.3629952	s	2.1089848077489513	V	40.250328215062694	Vs	-3.7	‰	-3.762294078477717	‰
42	10	MX018-1	Unknown	10		668.8	s	14.002995199999987	s	2.5024331887579097	V	6.5476439531591826	Vs	-28.363534678758629	‰	-28.391699664793585	‰
43	11	MX018-1	Unknown	11		686.3560064	s	14.212006399999995	s	4.7522837612124365	V	11.75211527130377	Vs	-27.959058875616783	‰	-27.987783570235933	‰
44	12	MX018-1	Unknown	12		707.6740096	s	7.31499511999995985	s	4.4493447715718268	V	11.220455626283002	Vs	-27.777027456627579	‰	-27.806004044059623	‰
45	13	MX018-1	Unknown	13		711.0180096	s	5.6430080000000089	s	0.43399684946379696	V	0.961699481614554	Vs	-32.982664556443389	‰	-33.004437648021451	‰
46	14	MX018-1	Unknown	14		767.6569984	s	16.301990400000022	s	3.7963876144467008	V	12.699624015797934	Vs	-13.589334611760485	‰	-13.637943952038334	‰
47	15	MX018-1	Unknown	15		816.9810048	s	15.675008000000048	s	3.2353982580247553	V	11.776251237025134	Vs	-27.848210770280545	‰	-27.877088855128768	‰
48	16	MX018-1	Unknown	16		861.08	s	15.675007999999934	s	2.6420021702509509	V	10.178447921744036	Vs	-29.419307075899681	‰	-29.446011097226624	‰
49	17	MX018-1	Unknown	17		1302.2790016	s	22.362995199999887	s	2.1091102591782533	V	40.090988043841918	Vs	-3.7	‰	-3.762294078477717	‰
50	18	MX018-1	Unknown	18		1352.648	s	22.362995199999887	s	2.1115093188101324	V	40.2156331730146	Vs	-3.6927708634734158	‰	-3.7550749455403185	‰
51	19	MX018-1	Unknown	19		1402.3900032	s	22.572006400000191	s	2.1109186532390716	V	40.248074004554738	Vs	-3.7440564811306309	‰	-3.8062895947978781	‰
52	1	MX018-1	Unknown	1		48.6969984	s	22.571993600000003	s	2.1138592042654332	V	40.199061855058922	Vs	-3.528933167441375	‰	-3.5914741013319813	‰
53	2	MX018-1	Unknown	2		98.4389888	s	22.5719936	s	2.1170667786609303	V	40.37664496735578	Vs	-3.649209189276803	‰	-3.7115735514464965	‰
54	3	MX018-1	Unknown	3		147.7629952	s	22.572006399999992	s	2.1135404702107721	V	40.330890824428067	Vs	-3.7655472327445816	‰	-3.8277506077771175	‰
55	4	MX018-1	Unknown	4		198.1319936	s	22.363008000000008	s	2.1144347484842396	V	40.344361680030715	Vs	-3.7873352972539465	‰	-3.8495085222338856	‰
56	5	MX018-1	Unknown	5		247.8739968	s	22.3629952	s	2.1128677645121581	V	40.277910714404513	Vs	-3.8090268593483634	‰	-3.8711700678145466	‰
57	6	MX018-1	Unknown	6		297.616	s	22.571993599999985	s	2.1142548593326969	V	40.303770739274405	Vs	-3.7948412564333678	‰	-3.8570040947603781	‰
58	7	MX018-1	Unknown	7		347.5669888	s	22.571993599999985	s	2.1134676425384349	V	40.296029016940359	Vs	-3.8301796449795589	‰	-3.8922935824841534	‰
59	8	MX018-1	Unknown	8		397.0999936	s	22.572006399999964	s	2.1119434796693839	V	40.254678848990736	Vs	-3.8379130884776957	‰	-3.9000163245393913	‰
60	9	MX018-1	Unknown	9		447.0509952	s	22.572006399999964	s	2.1105618056477895	V	40.217158449337695	Vs	-3.7	‰	-3.762294078477717	‰
61	10	MX018-1	Unknown	10		667.9639936	s	13.793996800000059	s	2.1931157544711368	V	5.5487623913287738	Vs	-28.189995244019329	‰	-28.218400371765025	‰
62	11	MX018-1	Unknown	11		685.52	s	12.121996800000034	s	3.546867793352146	V	8.60540497309292	Vs	-27.829329957168468	‰	-27.858234169050974	‰
63	12	MX018-1	Unknown	12		706.8379904	s	8.9869952000000239	s	3.3913226556432097	V	8.43728787774864	Vs	-27.835846225450879	‰	-27.864741420202407	‰
64	13	MX018-1	Unknown	13		710.6	s	5.642995199999973	s	0.37360212016964783	V	0.90622342022057645	Vs	-29.747935822968973	‰	-29.774185091924277	‰
65	14	MX018-1	Unknown	14		766.6119936	s	15.675007999999934	s	3.1973427423433893	V	10.234397955127406	Vs	-13.561224243801462	‰	-13.609872482856764	‰
66	15	MX018-1	Unknown	15		816.1449984	s	15.256998399999929	s	2.8370777548803292	V	9.7986703614597648	Vs	-27.69582789133651	‰	-27.724916841717678	‰
67	16	MX018-1	Unknown	16		860.452992	s	16.093004799999903	s	2.5138174228054013	V	8.9579352016910558	Vs	-29.4421533542083	‰	-29.468825761139556	‰
68	17	MX018-1	Unknown	17		1302.6969984	s	22.362995200000114	s	2.1089672293610406	V	40.13150372661714	Vs	-3.7	‰	-3.762294078477717	‰
69	18	MX018-1	Unknown	18		1352.648	s	22.362995200000114	s	2.1120488172951148	V	40.201507770752286	Vs	-3.68752005800721	‰	-3.749831406073390	‰
70	19	MX018-1	Unknown	19		1402.3899904	s	22.362995200000114	s	2.1096280095086435	V	40.185949608094973	Vs	-3.8091551146243185	‰	-3.8712981456124465	‰

Data Report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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:
AT% 13C/12C
AT% 13C/12C Unit
AT% 18O/16O
AT% 18O/16O Unit
Compound Name
d 13C/12C
d 13C/12C (ext. ref.)
d 13C/12C (ext. ref.) Unit
d 13C/12C Unit
d 17O/16O
d 17O/16O Unit
d 18O/16O
d 18O/16O Unit
d 45CO2/44CO2
d 45CO2/44CO2 Unit
d 46CO2/44CO2
d 46CO2/44CO2 Unit
Delta Calculation
Filename
Is selectable as Standard Peak
Is Square Peak
Is Standard Peak
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Peak Area 46.00 m/z
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Merge
Format
Calculations
Name
Caption
Repeat
Visible
Width
Column
Separator
Column
Text
Use for label
Peak Number
Peak ID
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Retention Time
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50.00 pt
f2
Peak Background 44.00 m/z
BGD 44 m/z [V]
50.00 pt
f3
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Area 44 m/z [Vs]
50.00 pt
f3
d 13C/12C
δ13C [‰]
50.00 pt
f2
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δ13C [‰] (Ext.Ref. Corr.)
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f2
d 18O/16O
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f2
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Name
Operator
Condition
Compound Name
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Label
is in list
Solvent
MX018-1
MX018-2
F1_QCN_11-Keto
F2_QCN_Testo

Data Report

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

QTEGRA

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

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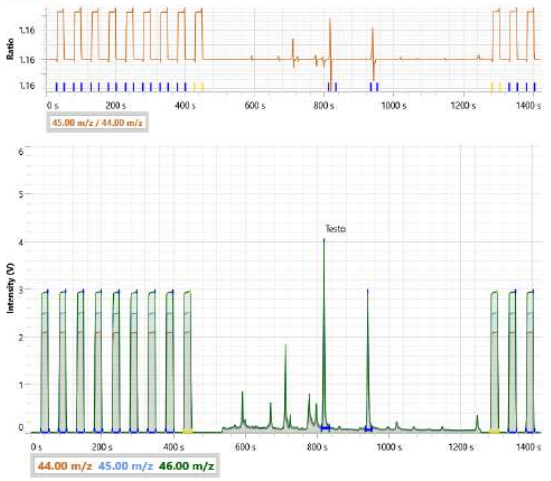
GC Report
9/18/2023 12:24:32 PM

QTEGRA

LabBook Steroids_13C_PTV LVI_DB35MS_AuxGas inGC - Sintered liner - 25ul - 20230201 - KCL - B01 - QCs.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

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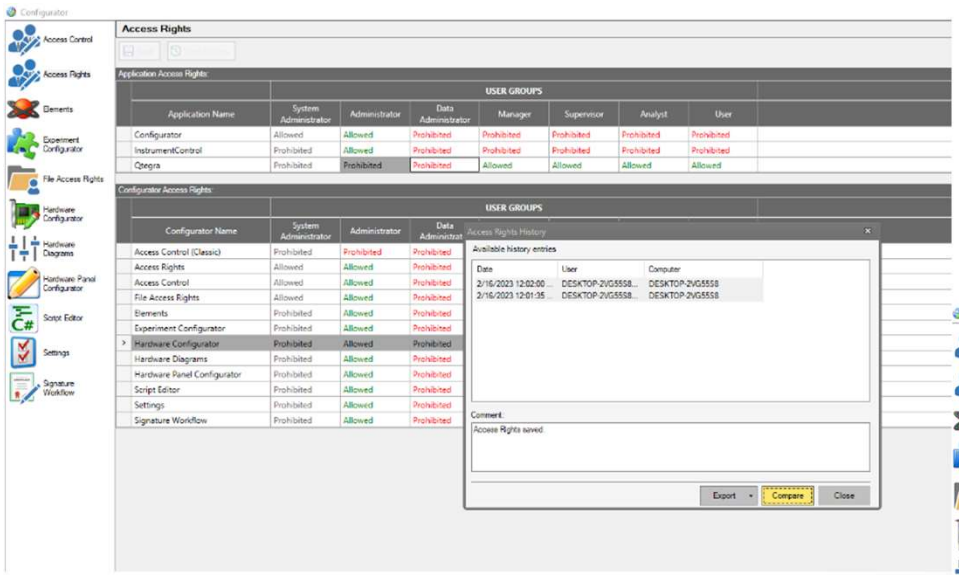
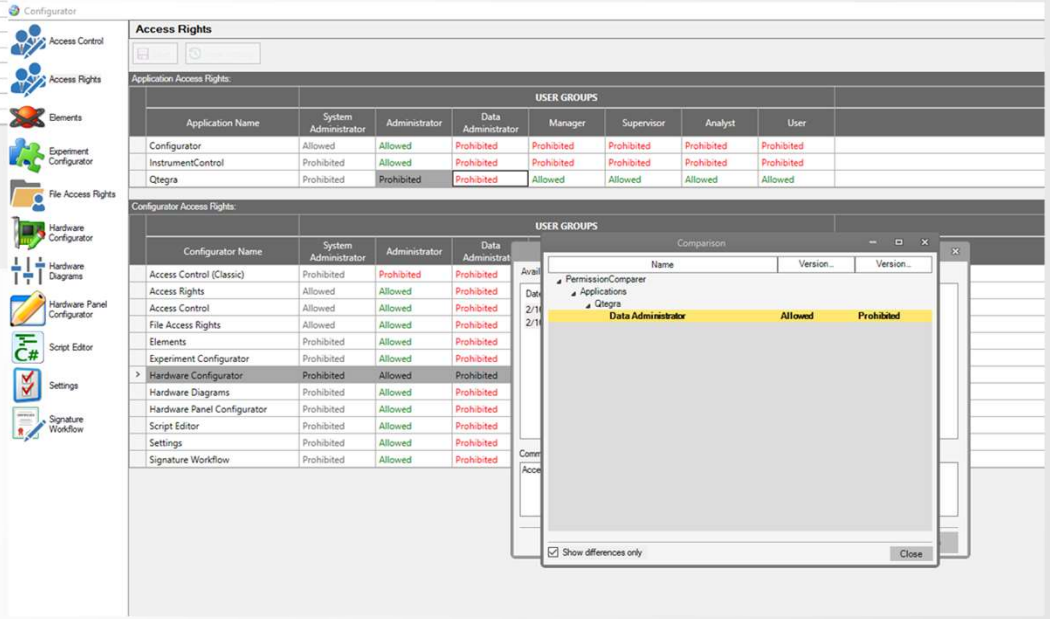
Data Integrity / Access Control

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

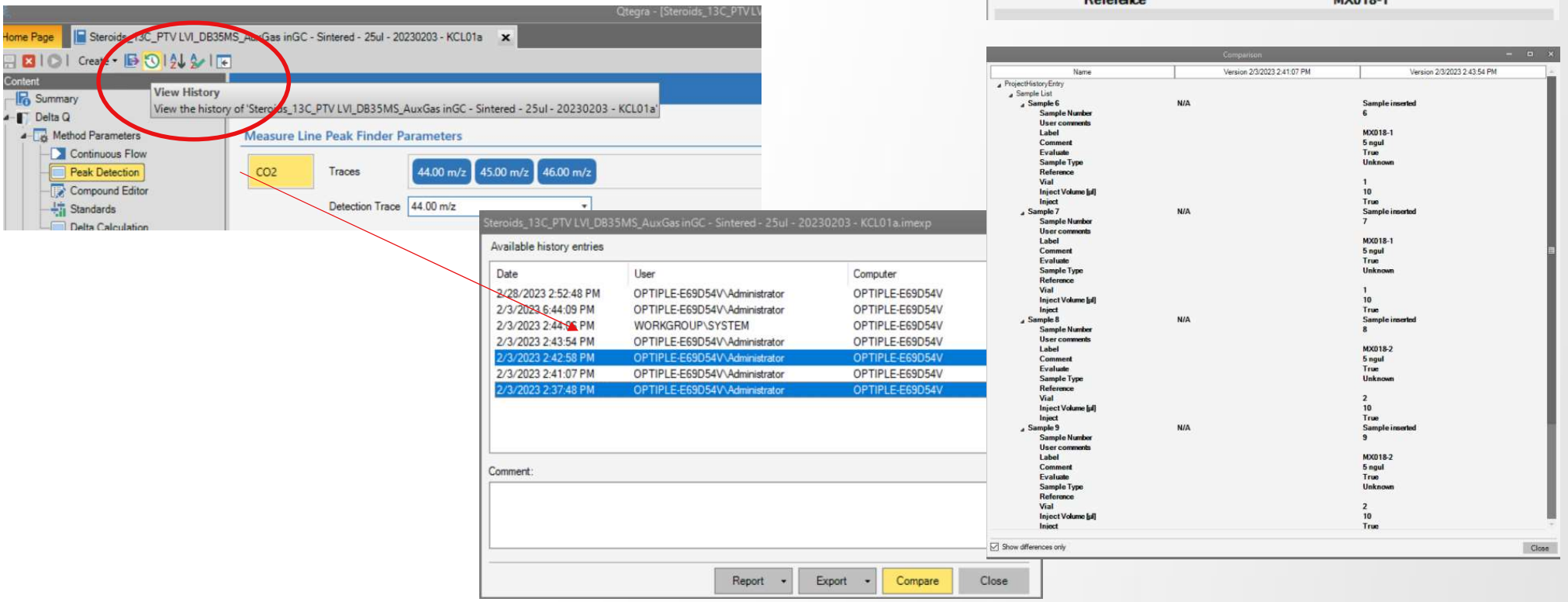
Data Integrity / Access rights





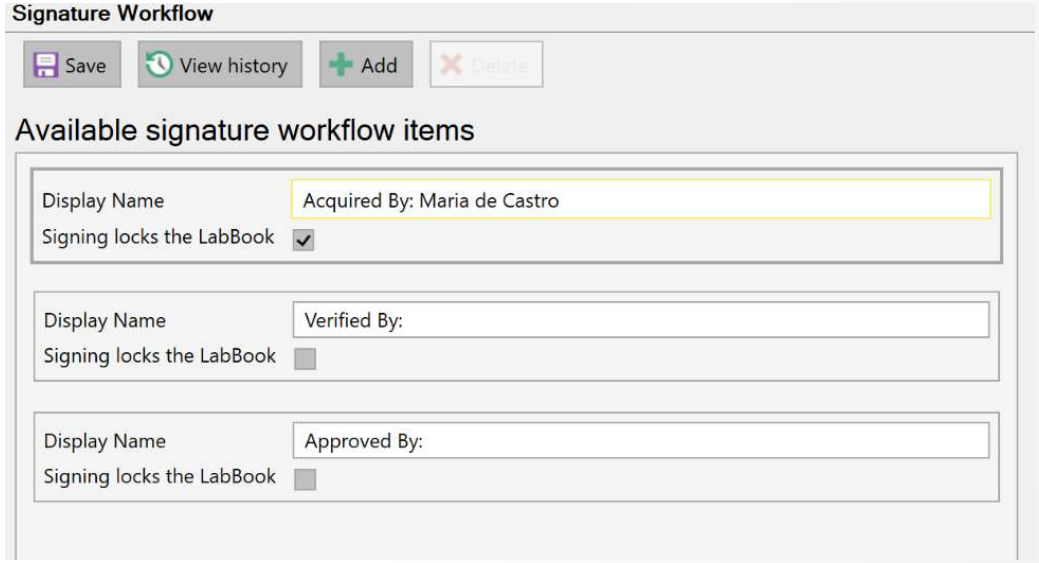
View history

LabBook changes history login



mario.tuthorn@thermofisher.com

Digital Signature



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