

Discover the Gold Standard for Dioxin Analysis



Thermo Scientific™ DFS™ Magnetic Sector GC-HRMS



ThermoFisher
S C I E N T I F I C

Latest News and Updates on DFS Magnetic Sector GC- HRMS

Heinz Mehlmann, Dirk Krumwiede

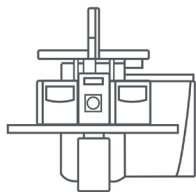
The world leader in serving science

- Projects we are currently working on.

- **Software**

- Instrument Control

- Target Quan



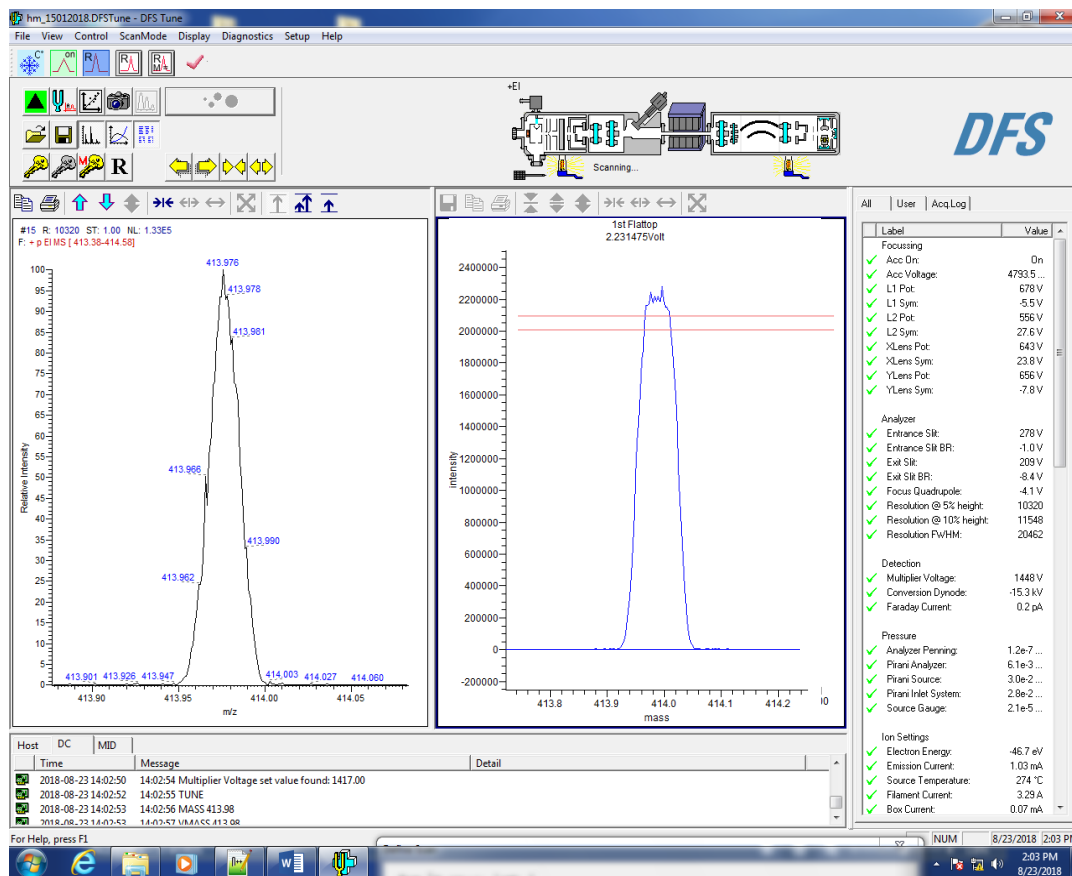
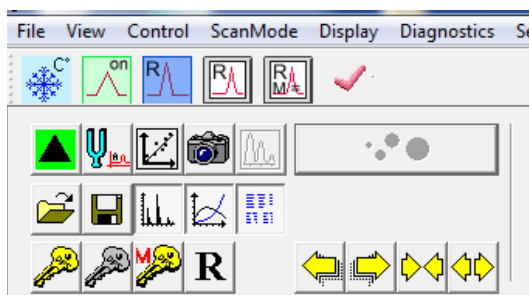
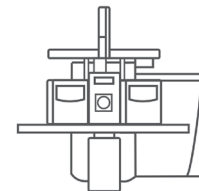
- **DualData XL**

- Additional Features



Instrument Software

- Improved MID process, faster section (window) changeover
- Smart MID
- Sequence Parameter logging.
- Function buttons.
- Automatic Resolution Setting.



MID (Multi Ion Detection)

- Example MID Sections
- Section for Tetra DF and Penta-, Hexa- PCBs

The screenshot shows the 'MID Dialog' software interface. The 'Run Settings' section is active, displaying the file path 'C:\calibur\data\hm_Japan_Prep_Jan2016\WF_06.raw'. The 'Segment Settings' section shows 'Times' with 'Start [min]: 17.15', 'End [min]: 23.00', 'Measure [min]: 5.85', and 'Cycle [sec]: 0.93'. A table with 19 rows and 8 columns is displayed. The columns are: Section 2, L/C, Mass, Gr., Int., Time[ms], Compound, and Comment. The table contains data for various compounds including PFK, TeCDF, 13C-TeCDF, TCDD, PeCB, 13C-TCDD, 13C-PeCB, HxCB, and 13C-HxCB. A status bar at the bottom shows '16' and '0.00000'. The interface includes a 'Close' button and a 'Help' button.

Section 2	L/C	Mass	Gr.	Int.	Time[ms]	Compound	Comment
1	Lock	292.98189	1	15	4	PFK	C7F11+
2		303.90160	1	1	63	TeCDF	M+
3		305.89870	1	1	63	TeCDF	(M+2)+
4		315.94190	1	2	31	13C-TeCDF	M+
5		317.93890	1	2	31	13C-TeCDF	(M+2)+
6		319.89650	1	1	63	TCDD	M+
7		321.89360	1	1	63	TCDD	(M+2)+
8		325.88040	1	1	63	PeCB	(M+2)+
9		327.87750	1	1	63	PeCB	(M+4)+
10	Cali	330.97869	1	15	4	PFK	C7F13+
11		331.93680	1	2	31	13C-TCDD	M+
12		333.93390	1	2	31	13C-TCDD	(M+2)+
13		337.92070	1	2	31	13C-PeCB	(M+2)+
14		339.91780	1	2	31	13C-PeCB	(M+4)+
15		359.84150	1	1	63	HxCB	(M+2)+
16		361.83850	1	1	63	HxCB	(M+4)+
17		371.88170	1	2	31	13C-HxCB	(M+2)+
18		373.87880	1	2	31	13C-HxCB	(M+4)+
19		0.00000	0	0	0		

MID (Multi Ion Detection)

Tune view

Locking is the critical step

Chromatogram

1. locking

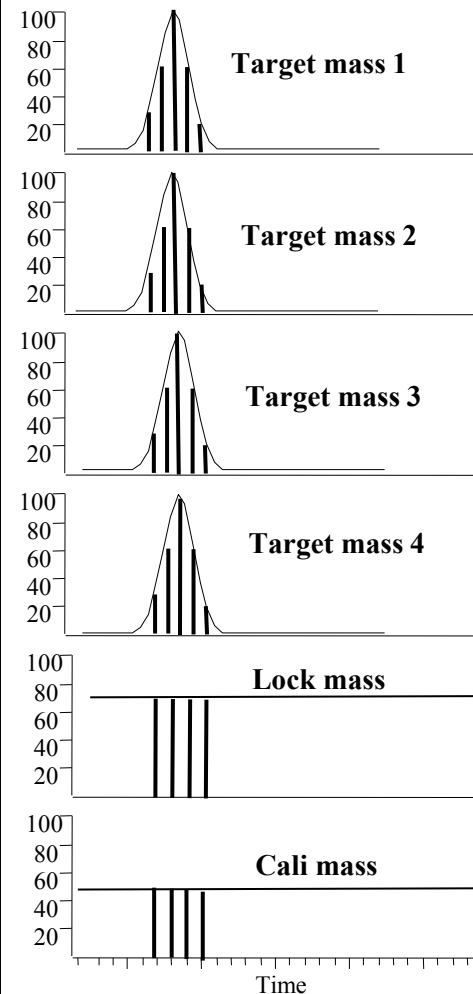
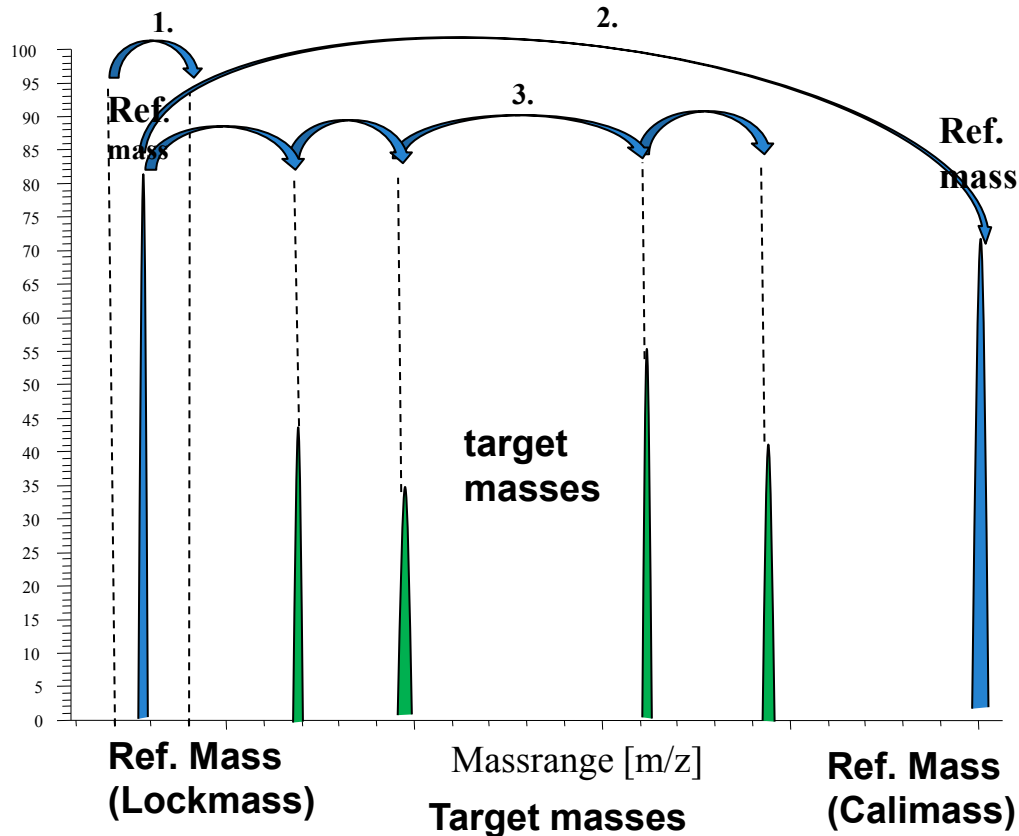
1st. Cycle

2. elec. jump to cali mass and calibration

3. elec. jump to target masses

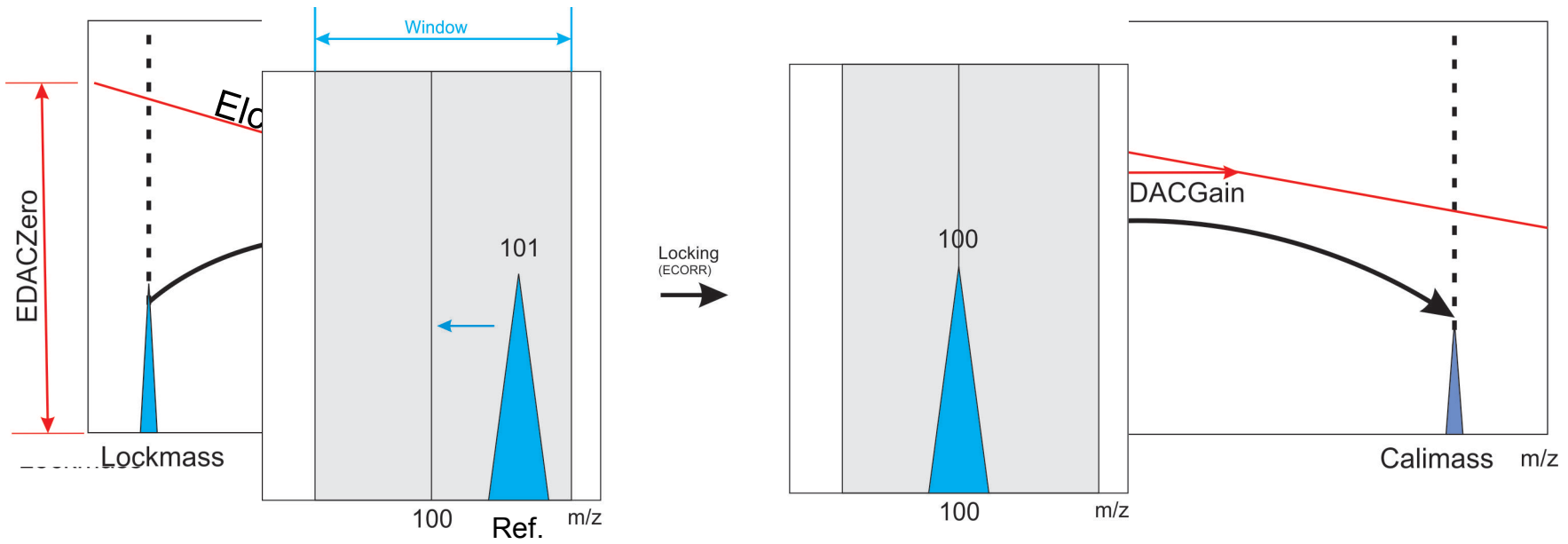
2nd. Cycle

3rd. Cycle



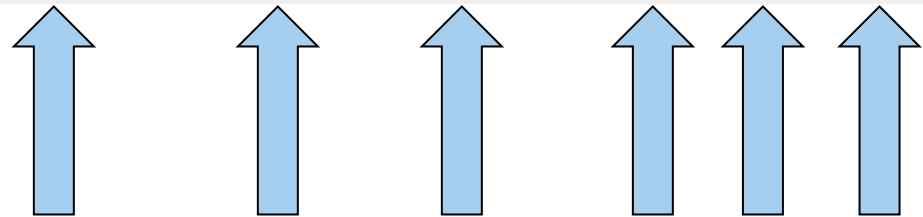
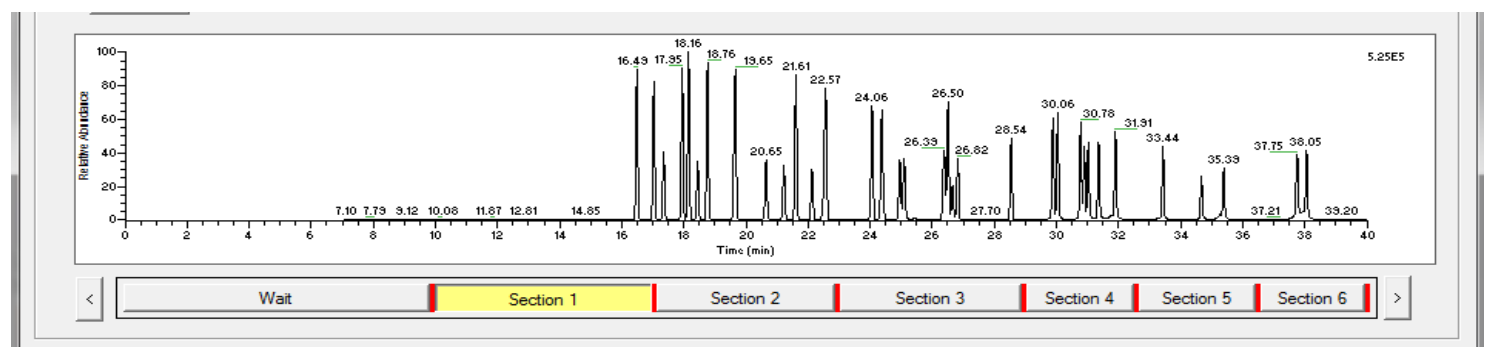
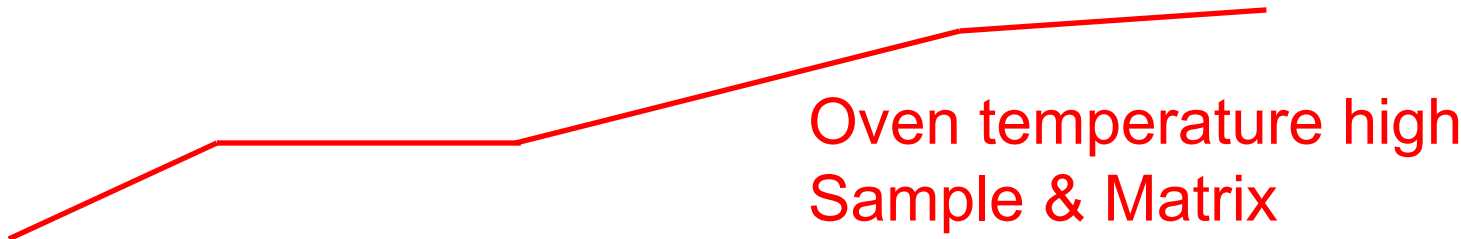
Smart Locking

- Standard Locking Process



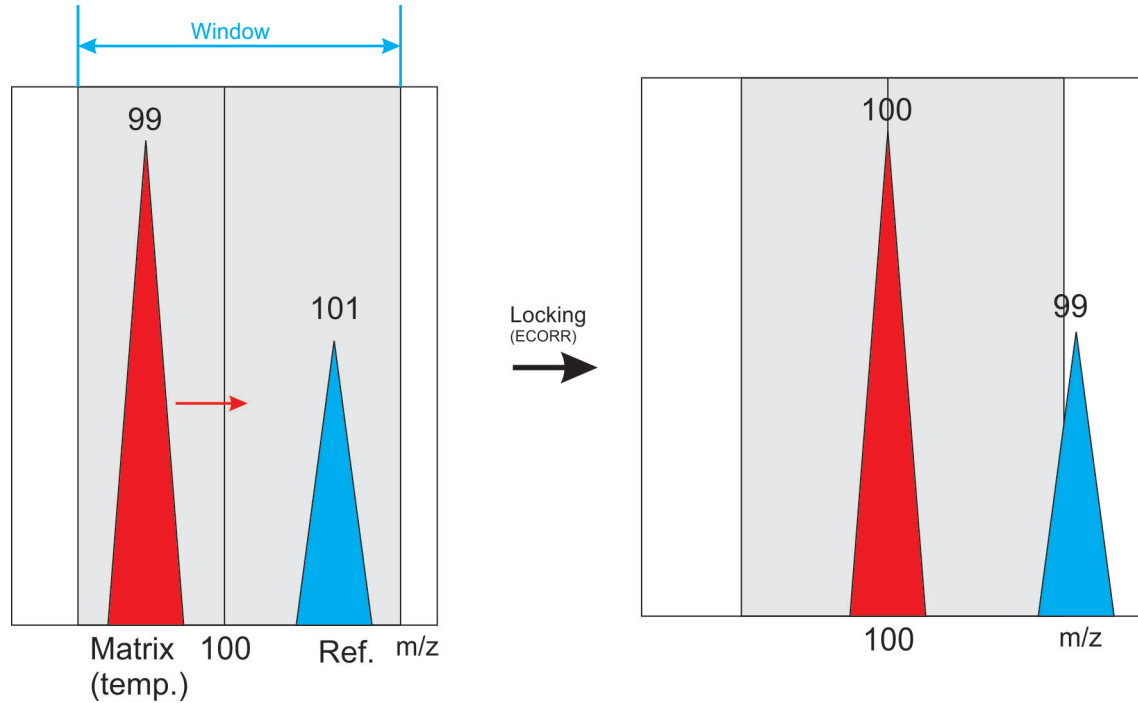
Smart Locking

- Standard Locking Process
- High chance of matrix interference



Smart Locking

- Matrix can disturb the Locking Process

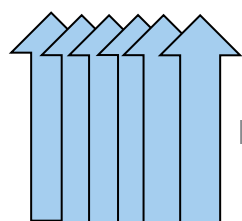
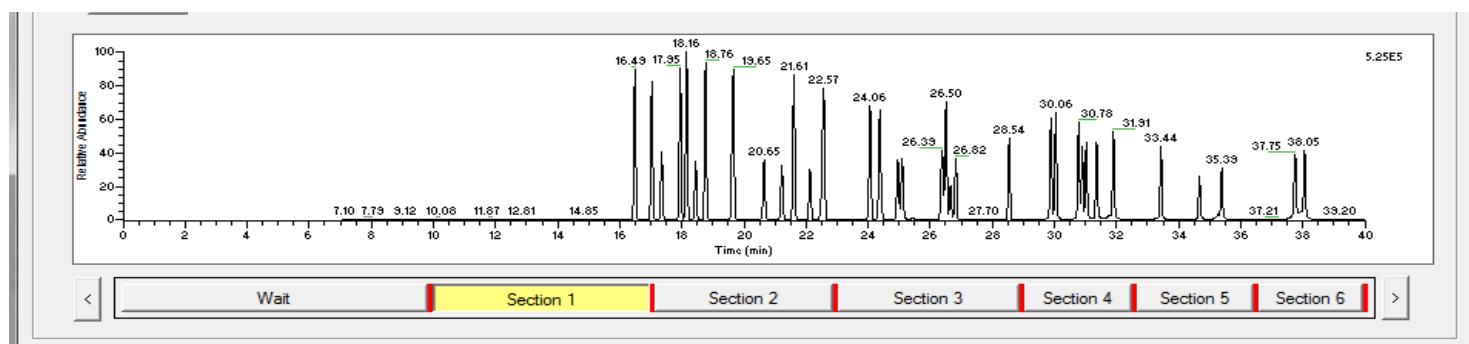


Smart Locking

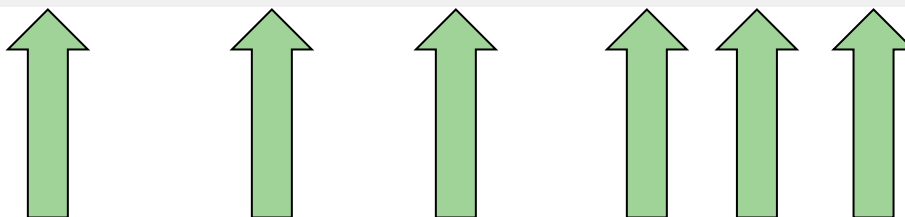
- Smart Locking Process
- Determination of the calibration parameters are done before injection.
- Low chance of matrix interference during calibration determination.

Oven temperature low
No Sample & Matrix

Oven temperature high
Sample & Matrix

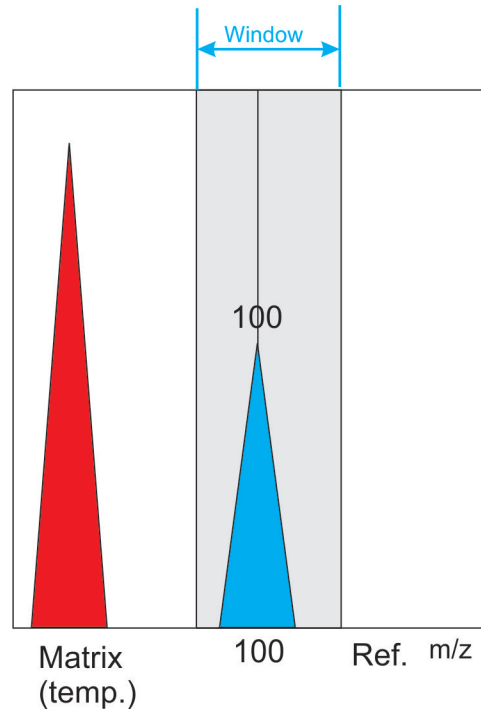


ECORR, EDACGain, EDACZero values



Smart Locking

- Locking during the measurement based on predefined parameters
- Matrix effects does not effect the calibration process during the run.



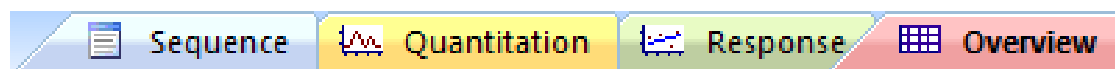
New Key features in TQ-DFS Magnetic Sector GC-HRMS:



- New Tab and features for overview table view
- Ability to process active (unfinished) sequences
- Changes for Noise determination and Detection/Quantitation Limit
- New Parameters for the different TEF and TEQ Systems with corresponding upper, medium and lower bound values

TargetQuan for DFS Magnetic Sector GC-HRMS: New tab and functions for Overview

- TargetQuan for DFS Magnetic Sector GC-HRMS



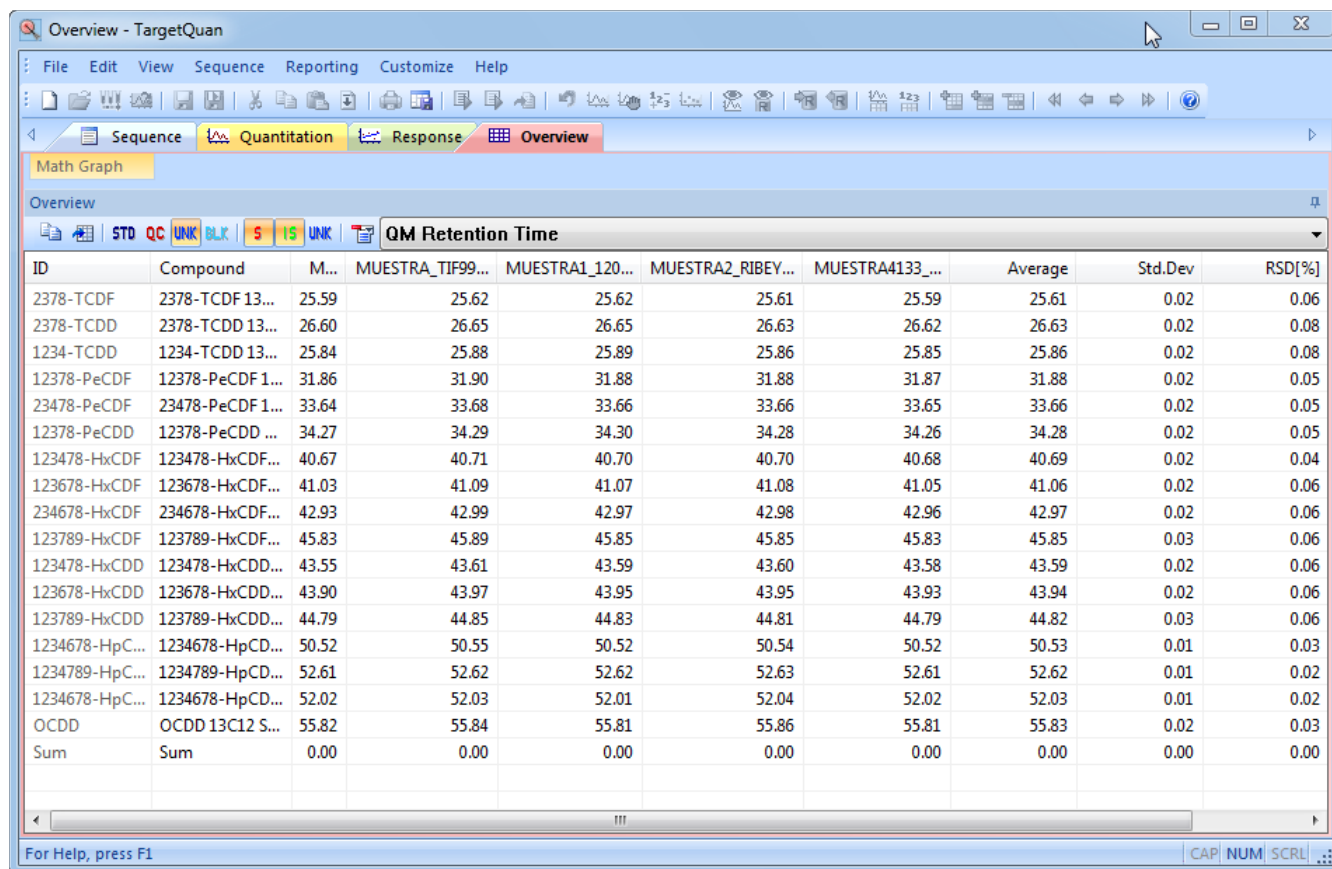
- Overview function was moved to a new Tab



- New filter function for recovery standards, internal standards and native compounds
- A graph view was added

TargetQuan for DFS Magnetic Sector GC-HRMS: New tab and functions for Overview

Displays the Retention times from all Internal Standards of all samples (unknowns) in a sequence



The screenshot shows the TargetQuan software interface with the Overview tab selected. The table displays retention times for various compounds and samples. The table has columns for ID, Compound, M... (Mass), and several sample identifiers (MUESTRA_TIF99..., MUESTRA1_120..., MUESTRA2_RIBEY..., MUESTRA4133...), along with Average, Std.Dev, and RSD[%].

ID	Compound	M...	MUESTRA_TIF99...	MUESTRA1_120...	MUESTRA2_RIBEY...	MUESTRA4133...	Average	Std.Dev	RSD[%]
2378-TCDF	2378-TCDF 13...	25.59	25.62	25.62	25.61	25.59	25.61	0.02	0.06
2378-TCDD	2378-TCDD 13...	26.60	26.65	26.65	26.63	26.62	26.63	0.02	0.08
1234-TCDD	1234-TCDD 13...	25.84	25.88	25.89	25.86	25.85	25.86	0.02	0.08
12378-PeCDF	12378-PeCDF 1...	31.86	31.90	31.88	31.88	31.87	31.88	0.02	0.05
23478-PeCDF	23478-PeCDF 1...	33.64	33.68	33.66	33.66	33.65	33.66	0.02	0.05
12378-PeCDD	12378-PeCDD ...	34.27	34.29	34.30	34.28	34.26	34.28	0.02	0.05
123478-HxCDF	123478-HxCDF...	40.67	40.71	40.70	40.70	40.68	40.69	0.02	0.04
123678-HxCDF	123678-HxCDF...	41.03	41.09	41.07	41.08	41.05	41.06	0.02	0.06
234678-HxCDF	234678-HxCDF...	42.93	42.99	42.97	42.98	42.96	42.97	0.02	0.06
123789-HxCDF	123789-HxCDF...	45.83	45.89	45.85	45.85	45.83	45.85	0.03	0.06
123478-HxCDD	123478-HxCDD...	43.55	43.61	43.59	43.60	43.58	43.59	0.02	0.06
123678-HxCDD	123678-HxCDD...	43.90	43.97	43.95	43.95	43.93	43.94	0.02	0.06
123789-HxCDD	123789-HxCDD...	44.79	44.85	44.83	44.81	44.79	44.82	0.03	0.06
1234678-HpC...	1234678-HpCD...	50.52	50.55	50.52	50.54	50.52	50.53	0.01	0.03
1234789-HpC...	1234789-HpCD...	52.61	52.62	52.62	52.63	52.61	52.62	0.01	0.02
1234678-HpC...	1234678-HpCD...	52.02	52.03	52.01	52.04	52.02	52.03	0.01	0.02
OCDD	OCDD 13C12 S...	55.82	55.84	55.81	55.86	55.81	55.83	0.02	0.03
Sum	Sum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

• Table view:

Selected
Parameter:

Quantitation Mass
Retention times

Selected Sample
Type Filter:

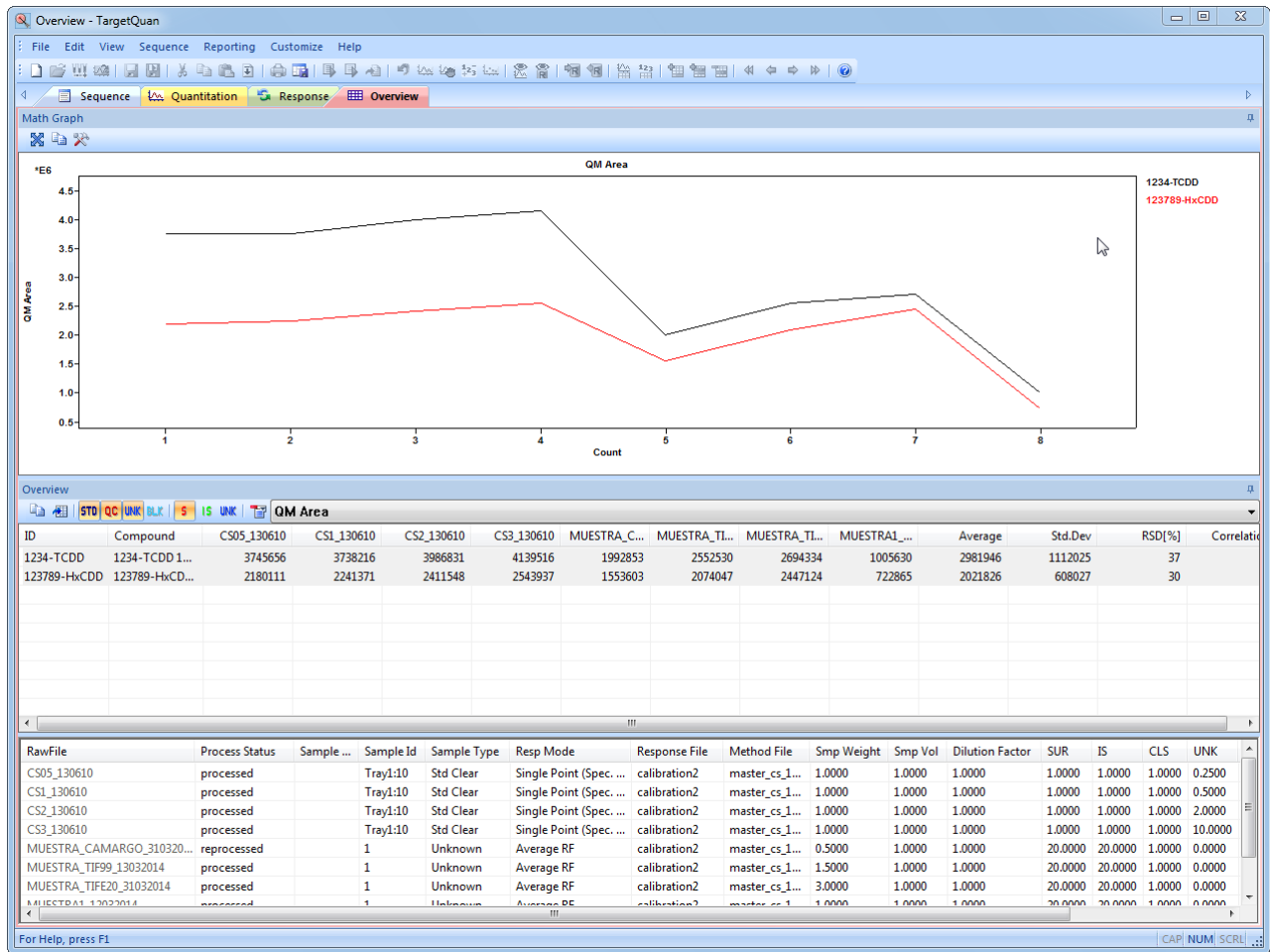
Unknowns

Selected Entry
Type Filter:

Internal standards

TargetQuan for DFS Magnetic Sector GC-HRMS: New tab and functions for Overview

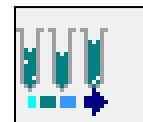
Displays the Quantitation Mass Area from the Recovery standards of Samples and Standards in a sequence



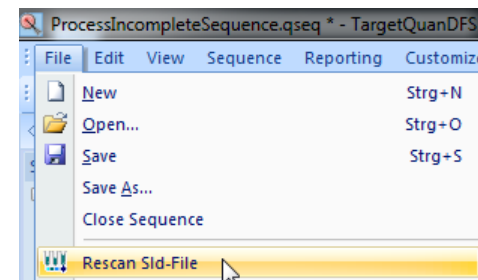
- Table view:
 - Selected Parameter: Quantitation Mass Area
 - Selected Sample Type Filter: Unknowns and Standards
 - Selected Entry Type Filter: Recovery Standards
- Graph view: Results of Recovery Standards

TargetQuan for DFS Magnetic Sector GC-HRMS: Processing of unfinished Sequences

	Sample Type	File Name	Path
1	Std Bracket	CS05_130610	F:\Targetquan\SequenceFolder
2	Std Bracket	CS1_130610	F:\Targetquan\SequenceFolder
3	Std Bracket	CS2_130610	F:\Targetquan\SequenceFolder
4	Std Bracket	CS3_130610	F:\Targetquan\SequenceFolder
5	Unknown	MUESTRA1_12032014	F:\Targetquan\SequenceFolder
6	Unknown	MUESTRA_TIF99_13032014	F:\Targetquan\SequenceFolder
7	Unknown	MUESTRA_TIFE20_31032014	F:\Targetquan\SequenceFolder
8	Unknown	MUESTRA_CAMARGO_31032014	F:\Targetquan\SequenceFolder



Rescan function :



ProcessIncompleteSequence.qseq * - TargetQuanDFS

File Edit View Sequence Reporting Customize Help

Sequence Quantitation Response Over

Setup

Global

Sequence File
Method Quan File
Response File
Xcalibur Sequence File
Raw Source Path
Report Layout
Export Layout(s)
Sum Area/Height Type
Limitcheck Dependency

	RawFile	Process Status
☑	CS05_130610	processed
	CS1_130610.raw	not processed
	CS2_130610.raw	not processed
	CS3_130610.raw	not processed
	MUESTRA1_12032014.raw	RawFile not valid
	MUESTRA_TIF99_13032014.raw	RawFile not valid
	MUESTRA_TIFE20_31032014.raw	RawFile not valid
	MUESTRA_CAMARGO_31032014.raw	RawFile not valid

ProcessIncompleteSequence.qseq * - TargetQuanDFS

File Edit View Sequence Reporting Customize Help

Sequence Quantitation Response Over

Setup

Global

Sequence File
Method Quan File
Response File
Xcalibur Sequence File
Raw Source Path
Report Layout
Export Layout(s)
Sum Area/Height Type
Limitcheck Dependency

	RawFile	Process Status
☑	CS05_130610	processed
☑	CS1_130610.raw	processed
☑	CS2_130610.raw	processed
☑	CS3_130610.raw	processed
	MUESTRA1_12032014.raw	not processed
	MUESTRA_TIF99_13032014.raw	not processed
	MUESTRA_TIFE20_31032014.raw	not processed
	MUESTRA_CAMARGO_31032014.raw	not processed

- Additional raw files are added to the TQ sequence has been measured
- New entries can be processed
- Note: Integration, etc. of previous processed entries are not changed
- Evaluation of calibration could be carried out

TargetQuan for DFS Magnetic Sector GC-HRMS: New Parameters for Noise and Quantitation Limit

Quan Parameter	
QualBrowser Compatibility	Compatibility off
Sum Area/Height	Sum QM RM1
Quantitation Status	Dependent on Area
TEQ on Area [hTOA]	Dependent on Area
Injection Volume [hIV]	1.0
Sample Volume [hSV]	1.0
Sample Weight [hSWT]	2.0
Dilution Factor [hDF]	1.0
Det. Limit Factor [hDLF]	3.0
Quan. Limit Factor [hQLF]	10.0
Noise Sigma [hSIG]	4
Response Factor Mode	Average RF
Fit Calc. Mode	Linear Fit
Regression Mode	Non weighted Regression
Weighted Regression Factor	1.0

- New Parameters:
 - Quantitation limit
 - Quantitation limit factor
 - Sigma factor for Noise

Entry	Compound Name	CAA Calculated Amount (A)	DLA Detection Limit (A)	QLA Quantitation Limit (A)
1	2378-TCDF	n.d. < 0.367	0.048	0.160
2	2378-TCDD	n.d. < 0.108	0.032	0.108
3	12378-PeCDF	0.199	0.054	0.180

Entry	Compound Name	CAA Calculated Amount (A)	DLA Detection Limit (A)	QLA Quantitation Limit (A)
1	2378-TCDF	8.922	0.211	0.703
2	2378-TCDD	n.d. < 0.374	0.112	0.374
3	12378-PeCDF	1.213	0.191	0.638



- **Noise Determination Methods**

- Automatic noise determination (algorithm is applied on the complete time range of measured mass trace, default method)

New:

- Automatic noise determination with pre-selected time range (for example 1 to 0.5 minutes before the peak)
- Manual noise range determination by selection of a time range in the chromatogram with the mouse

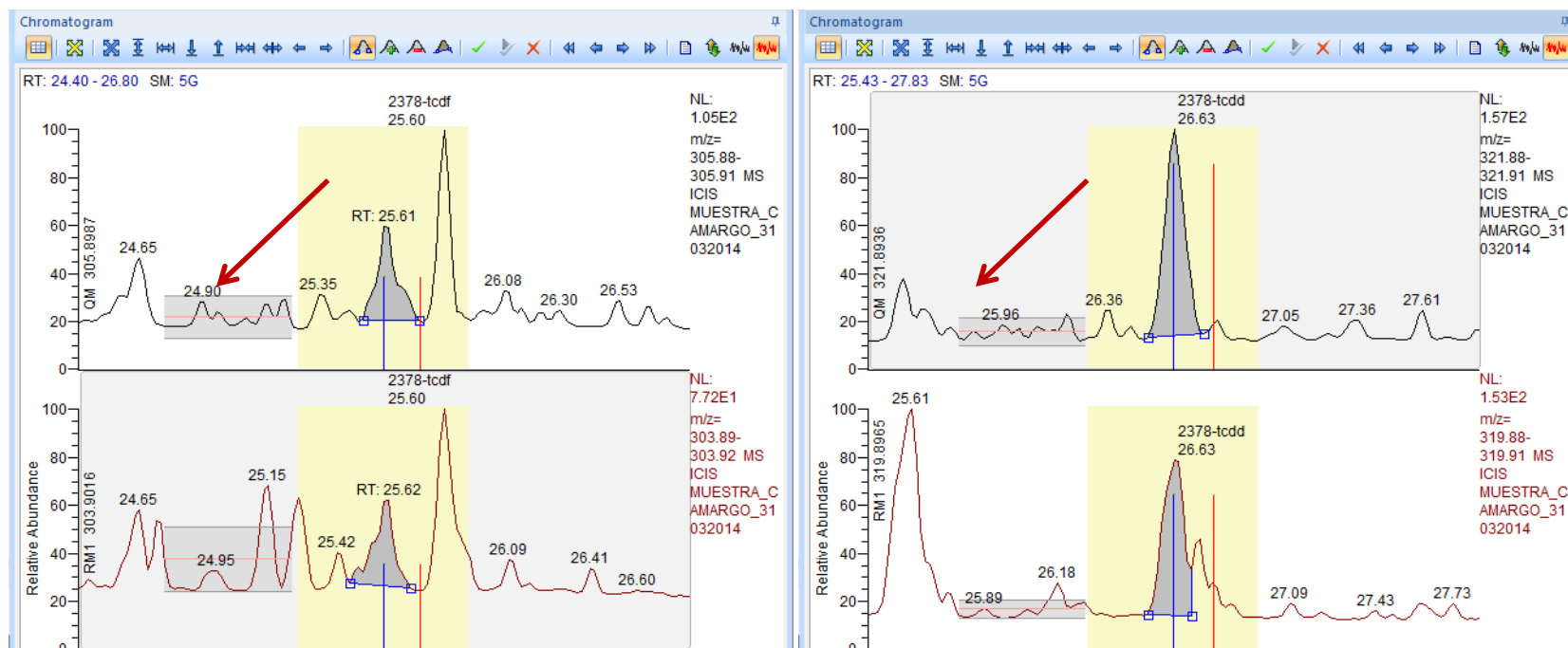
Automatic Noise determination with pre-selected time range

Entry	Entry Identifier	CAA	Noise Range	
		Calculated Amount (A)	QM	RM1
1	2378-tcdf	0.41	-1.00 - -0.50	-1.00 - -0.50
2	2378-tcdd	2.18	-1.00 - -0.50	-1.00 - -0.50
3	12378-pecdf	n.d. < 1.05	-1.00 - -0.50	-1.00 - -0.50
4	23478-pecdf	1.08	-1.00 - -0.50	-1.00 - -0.50
5	12378-pecdd	n.d. < 0.91	-1.00 - -0.50	-1.00 - -0.50
6	123478-hxcdf	n.d. < 0.52	-1.00 - -0.50	-1.00 - -0.50
7	123678-hxcdf	1.42	-1.00 - -0.50	-1.00 - -0.50
8	234678-hxcdf	0.51	-1.00 - -0.50	-1.00 - -0.50
9	123789-hxcdf	n.d. < 1.36	-1.00 - -0.50	-1.00 - -0.50
10	123478-hxcdd	n.d. < 1.40	-1.00 - -0.50	-1.00 - -0.50
11	123678-hxcdd	3.00	-1.00 - -0.50	-1.00 - -0.50
12	123789-hxcdd	n.d. < 0.60	-1.00 - -0.50	-1.00 - -0.50
13	1234678-hpcdf	2.51	-1.00 - -0.50	-1.00 - -0.50
14	1234789-hpcdf	n.d. < 0.29	-1.00 - -0.50	-1.00 - -0.50
15	1234678-hpcdd	18.81	-1.00 - -0.50	-1.00 - -0.50
16	ocdf	n.d. < 0.23	-1.00 - -0.50	-1.00 - -0.50
17	ocdd	41.54	-1.00 - -0.50	-1.00 - -0.50

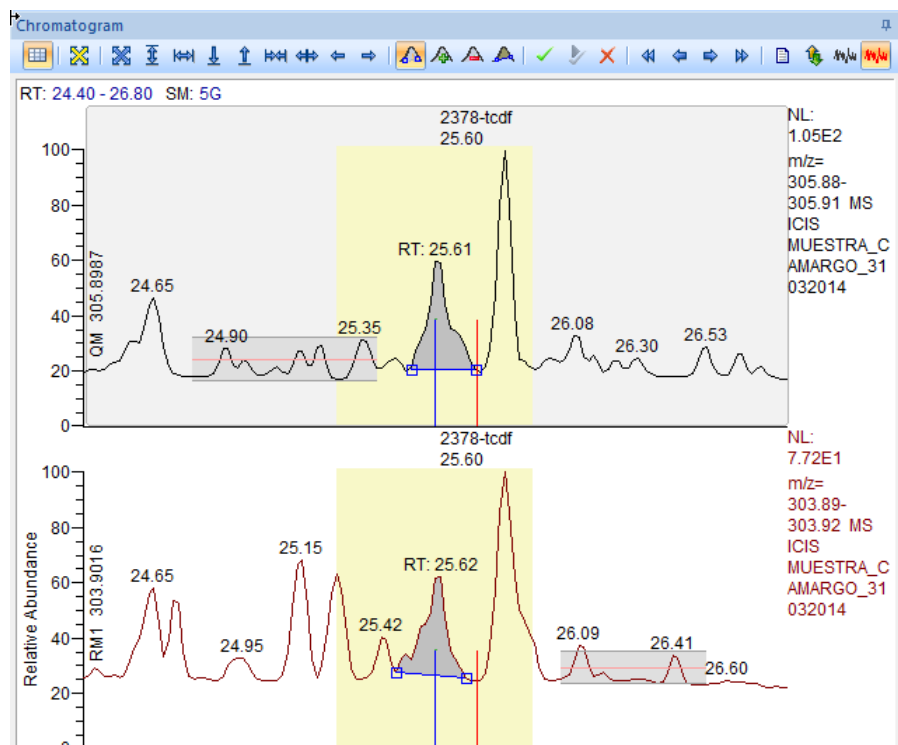
- User defined Noise Range for every entry:
- Noise Range Quantitation Mass
- Noise Range Ratio Mass
- In this example the defined range is 1 minute to 0.5 minutes before the Peak
- Range is displayed in the chromatograms

TargetQuan for DFS Magnetic Sector GC-HRMS: New Noise Features

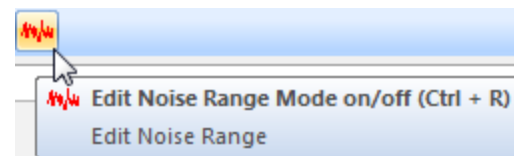
- Predefined Noise range (-1 min to -0.5 min) displayed in the chromatograms Example: TCDF and TCDD:



Manually selected time range for noise determination

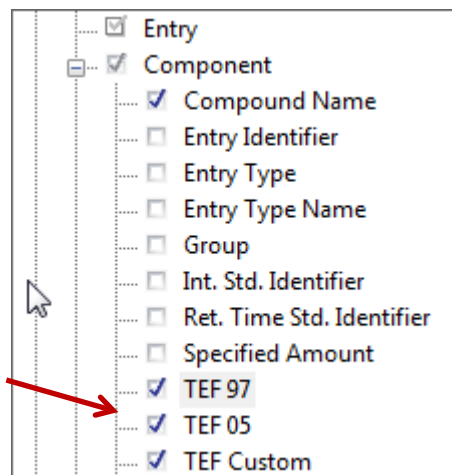


Entry	Entry Identifier	CAA Calculated Amount (A)	Noise Range QM	QM Noise	R1N RM1 Noise	S2NH S/N	QLA Quantitation Limit (A)
1	2378-tcdf	0.41	-0.97 - -0.34	8.26	4.50	5	0.2351



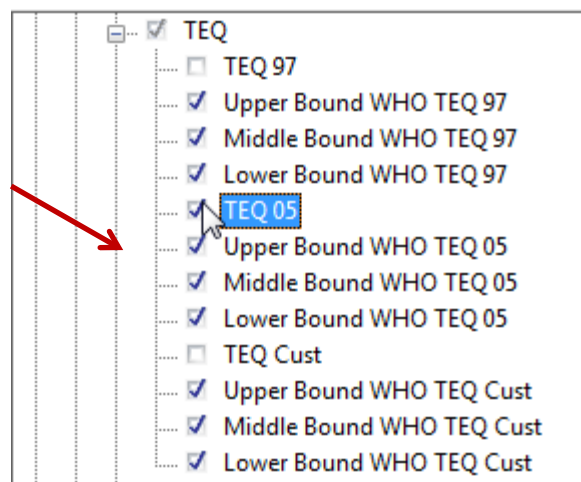
- Noise time range of Quan Mass and Ratio Mass are independent
- Ranges can be drawn where the most characteristic noise can be found

TargetQuan for DFS Magnetic Sector GC-HRMS: Additional TEF and TEQ Factors



New Parameters in TargetQuan:

- Additional TEF factors:
 - TEF 97: TEF WHO 1997 values
 - TEF 05: TEF WHO 2005 values
 - TEF Cust: for example TEF Nato values



- Corresponding TEQ values:

For example:

- TEQ 05
- Upper Bound WHO TEQ 05
- Medium Bound WHO TEQ 05
- Lower Bound WHO TEQ 05

Calculation of upper, middle and lower bound TEQ for the TEF system required by the method

Entry	Compound Name	CAA	QLA	TEF05	UTQ05	MTQ05	LQ05
		Calculated Amount (A)	Quantitation Limit (A)	TEF 05	Upper Bound WHO TEQ 05	Middle Bound WHO TEQ 05	Lower Bound WHO TEQ 05
1	2378-TCDF	0.409	0.3393	0.1000	0.0409	0.0409	0.0409
2	2378-TCDD	2.179	0.4135	1.0000	2.1790	2.1790	2.1790
3	12378-PeCDF	n.d. < 1.394	1.0499	0.0300	0.0315	0.0157	0.0000
4	23478-PeCDF	1.081	0.2846	0.3000	0.3242	0.3242	0.3242
5	12378-PeCDD	n.d. < 1.986	0.9143	1.0000	0.9143	0.4572	0.0000
6	123478-HxCDF	n.d. < 0.871	0.5240	0.1000	0.0524	0.0262	0.0000
7	123678-HxCDF	1.421	0.8611	0.1000	0.1421	0.1421	0.1421
8	234678-HxCDF	0.510	0.6256	0.1000	0.0510	0.0510	0.0510
9	123789-HxCDF	n.d. < 1.360	1.3602	0.1000	0.1360	0.0680	0.0000
10	123478-HxCDD	n.d. < 1.398	1.3985	0.1000	0.1398	0.0699	0.0000
11	123678-HxCDD	3.000	0.5326	0.1000	0.3000	0.3000	0.3000
12	123789-HxCDD	n.d. < 0.602	0.6016	0.1000	0.0602	0.0301	0.0000
13	1234678-HpCDF	2.510	0.2142	0.0100	0.0251	0.0251	0.0251
14	1234789-HpCDF	n.d. < 0.289	0.2886	0.0100	0.0029	0.0014	0.0000
15	1234678-HpCDD	18.807	0.4397	0.0100	0.1881	0.1881	0.1881
16	OCDF	n.d. < 0.231	0.2306	0.0003	0.0001	0.0000	0.0000
17	OCDD	41.539	0.3568	0.0003	0.0125	0.0125	0.0125
18	Sum	71.455	0.4519	0.0000	4.6000	3.9314	3.2628

Entry	Compound Name	CAA	QLA	TEF05	UTQ05	MTQ05	LQ05
		Calculated Amount (A)	Quantitation Limit (A)	TEF 05	Upper Bound WHO TEQ 05	Middle Bound WHO TEQ 05	Lower Bound WHO TEQ 05
1	Sum	71.455	0.4519	0.0000	4.6000	3.9314	3.2628

TargetQuan for DFS Magnetic Sector GC-HRMS: Additional TEF and TEQ Factors

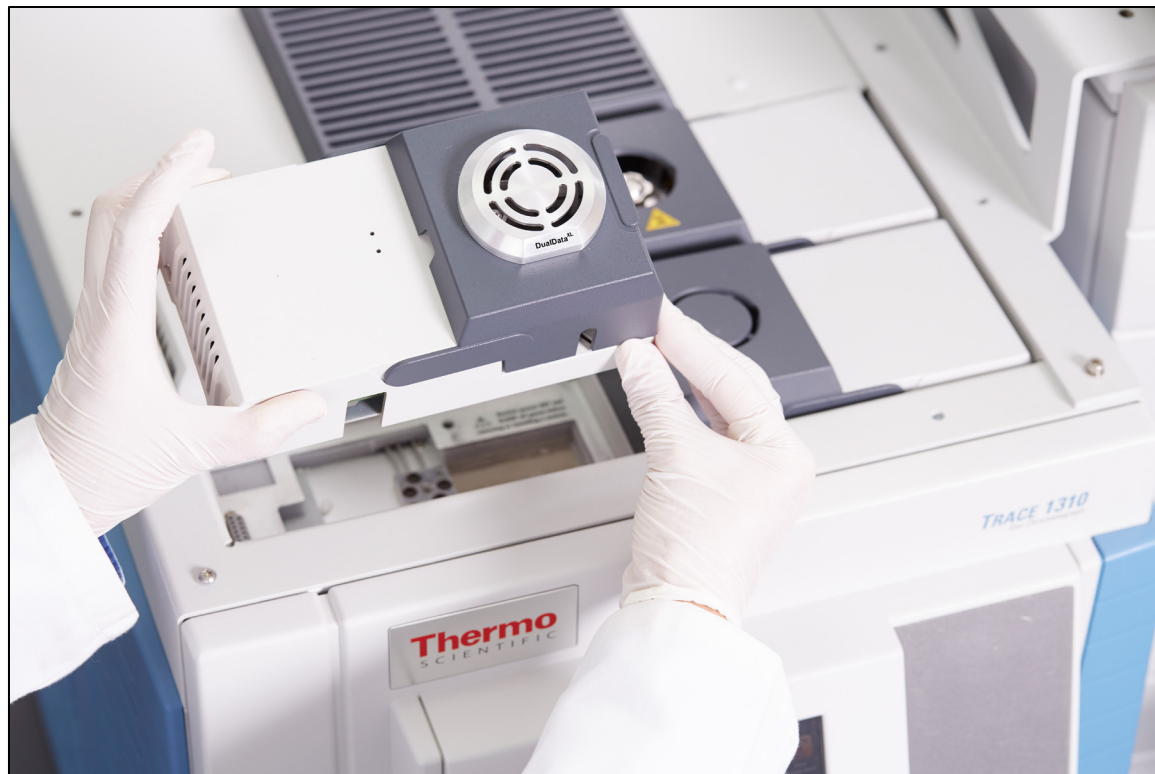
Calculation and Comparison of Upper Bound TEQs for different TEF Systems

Entry	Compound Name	CAA	QLA	TEF97	TEF05	TEFC	UTQ97	UTQ05	UTQC
		Calculated Amount (A)	Quantitation Limit (A)	TEF 97	TEF 05	TEF Custom	Upper Bound WHO TEQ 97	Upper Bound WHO TEQ 05	Upper Bound WHO TEQ Cust
1	2378-TCDF	0.41	0.2515	0.1000	0.1000	0.1000	0.0409	0.0409	0.0409
2	2378-TCDD	2.18	0.4538	1.0000	1.0000	1.0000	2.1790	2.1790	2.1790
3	12378-PeCDF	n.d. < 1.39	0.5796	0.0500	0.0300	0.0500	0.0290	0.0174	0.0290
4	23478-PeCDF	1.08	0.5876	0.5000	0.3000	0.5000	0.5403	0.3242	0.5403
5	12378-PeCDD	n.d. < 1.99	1.0887	1.0000	1.0000	0.5000	1.0887	1.0887	0.5443
6	123478-HxCDF	n.d. < 0.87	0.6174	0.1000	0.1000	0.1000	0.0617	0.0617	0.0617
7	123678-HxCDF	1.42	0.6323	0.1000	0.1000	0.1000	0.1421	0.1421	0.1421
8	234678-HxCDF	0.51	0.7380	0.1000	0.1000	0.1000	0.0510	0.0510	0.0510
9	123789-HxCDF	n.d. < 0.92	0.9228	0.1000	0.1000	0.1000	0.0923	0.0923	0.0923
10	123478-HxCDD	n.d. < 0.99	0.4725	0.1000	0.1000	0.1000	0.0472	0.0472	0.0472
11	123678-HxCDD	3.00	0.5005	0.1000	0.1000	0.1000	0.3000	0.3000	0.3000
12	123789-HxCDD	n.d. < 0.54	0.5410	0.1000	0.1000	0.1000	0.0541	0.0541	0.0541
13	1234678-HpCDF	2.51	0.3686	0.0100	0.0100	0.0100	0.0251	0.0251	0.0251
14	1234789-HpCDF	n.d. < 0.41	0.4101	0.0100	0.0100	0.0100	0.0041	0.0041	0.0041
15	1234678-HpCDD	18.81	0.6591	0.0100	0.0100	0.0100	0.1881	0.1881	0.1881
16	OCDF	n.d. < 0.51	0.5128	0.0001	0.0003	0.0010	0.0001	0.0002	0.0005
17	OCDD	41.54	0.7892	0.0001	0.0003	0.0010	0.0042	0.0125	0.0415
18	Sum	71.46	0.5534	0.0000	0.0000	0.0000	4.8478	4.6285	4.3413

	UTQ97	UTQ05	UTQC
Compound Name	Upper Bound WHO TEQ 97	Upper Bound WHO TEQ 05	Upper Bound WHO TEQ Cust
Sum	4.8478	4.6285	4.3413

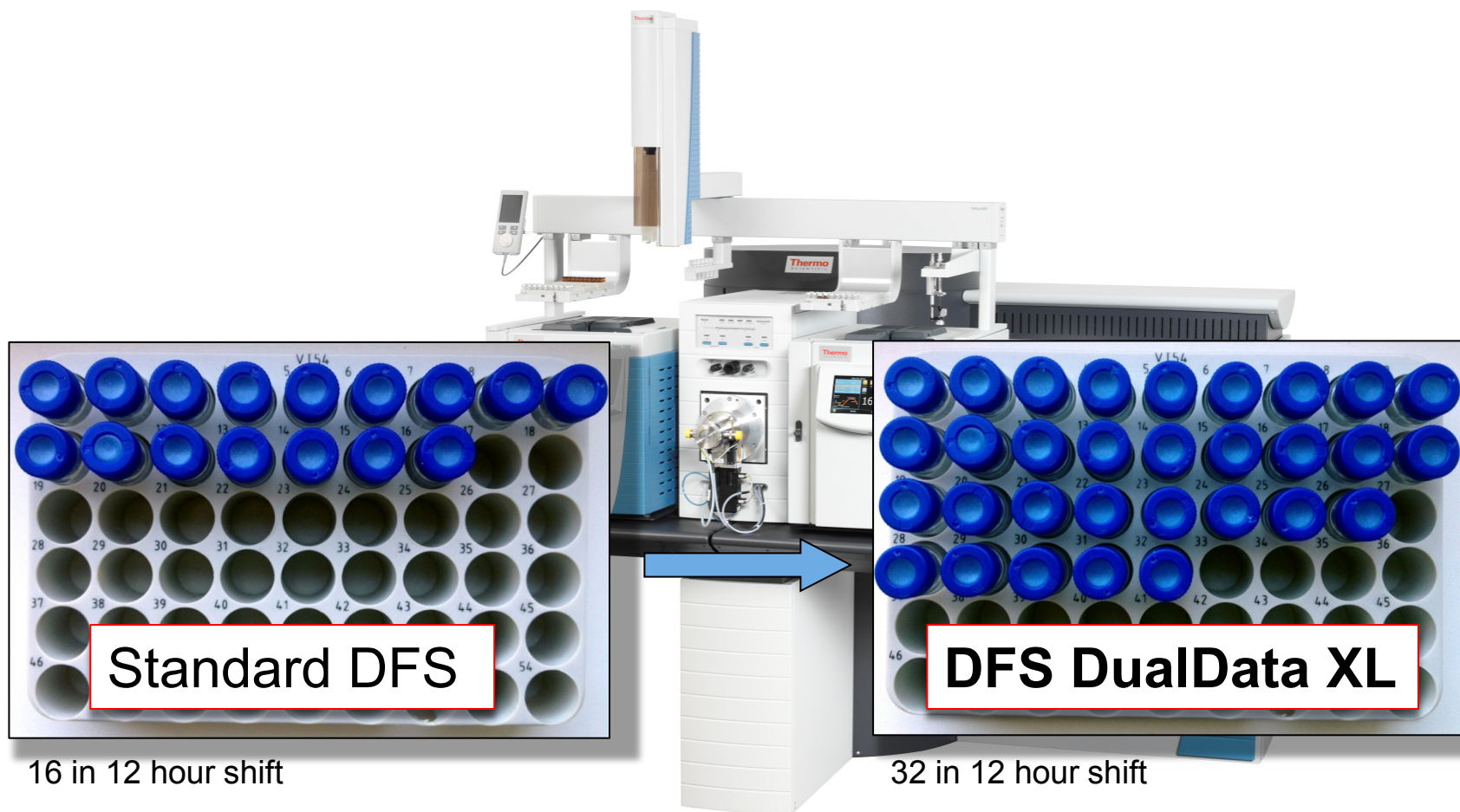
Dual Data XL: additional Features

- Column exchange without venting.
- Independent makeup- and column flow regulation.
- Dual column per GC setup using 5 port wafer.



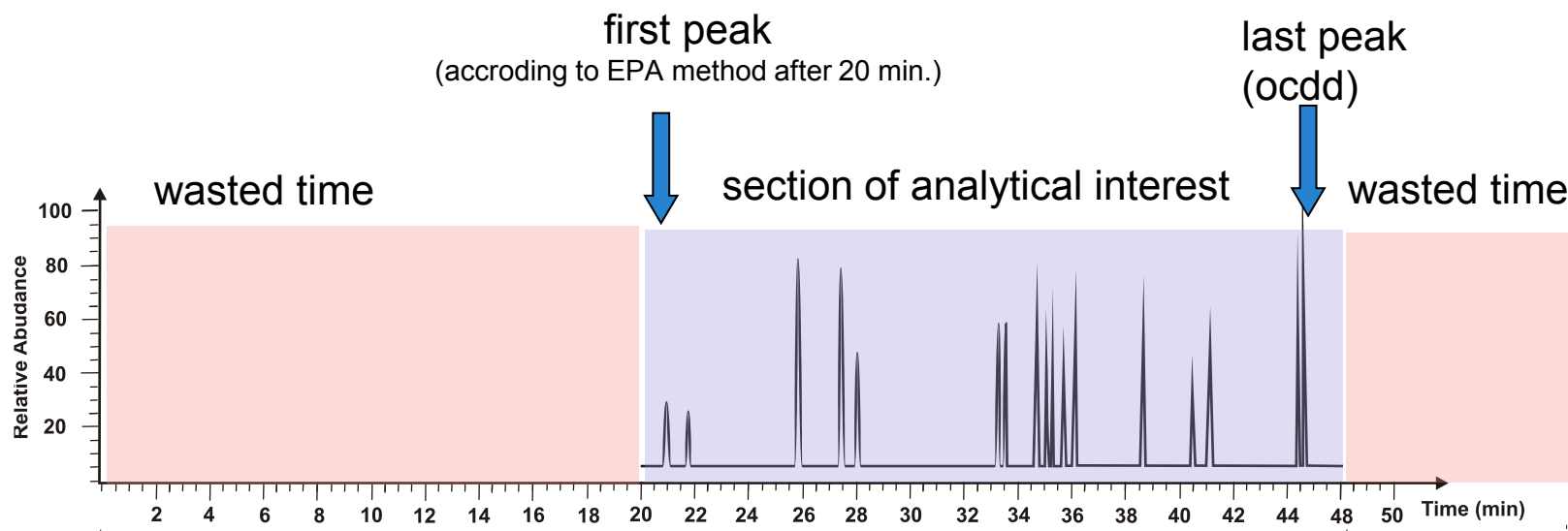
What is DFS Magnetic Sector GC-HRMS DualData XL ?

- Productivity: up to **2 times the number of samples** in the same timeframe.



DFS DualData XL: Background & Basic Idea

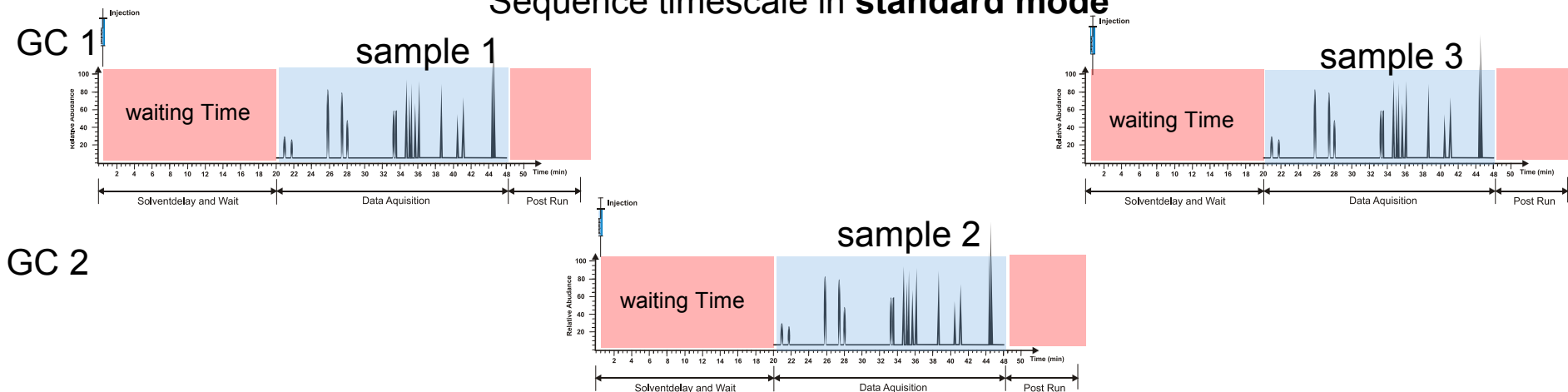
- Targeted Application: **Dioxins/Furans** following EPA 1613
- The first and last peak of a chromatogram defines the time section of analytical interest.



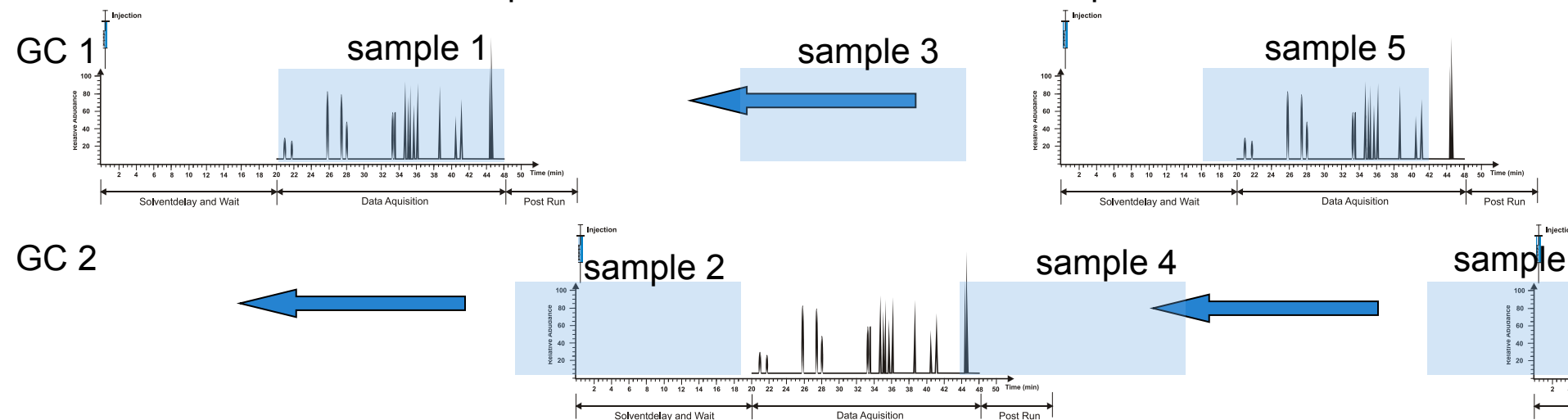
Chromatogram of a typical Dioxin run on a 60 meter column

Comparison: Standard DFS Magnetic Sector GC-HRMS vs. DFS Magnetic Sector GC-HRMS DualData XL

Sequence timescale in **standard mode**



Sequence timescale **with DualData XL** Option



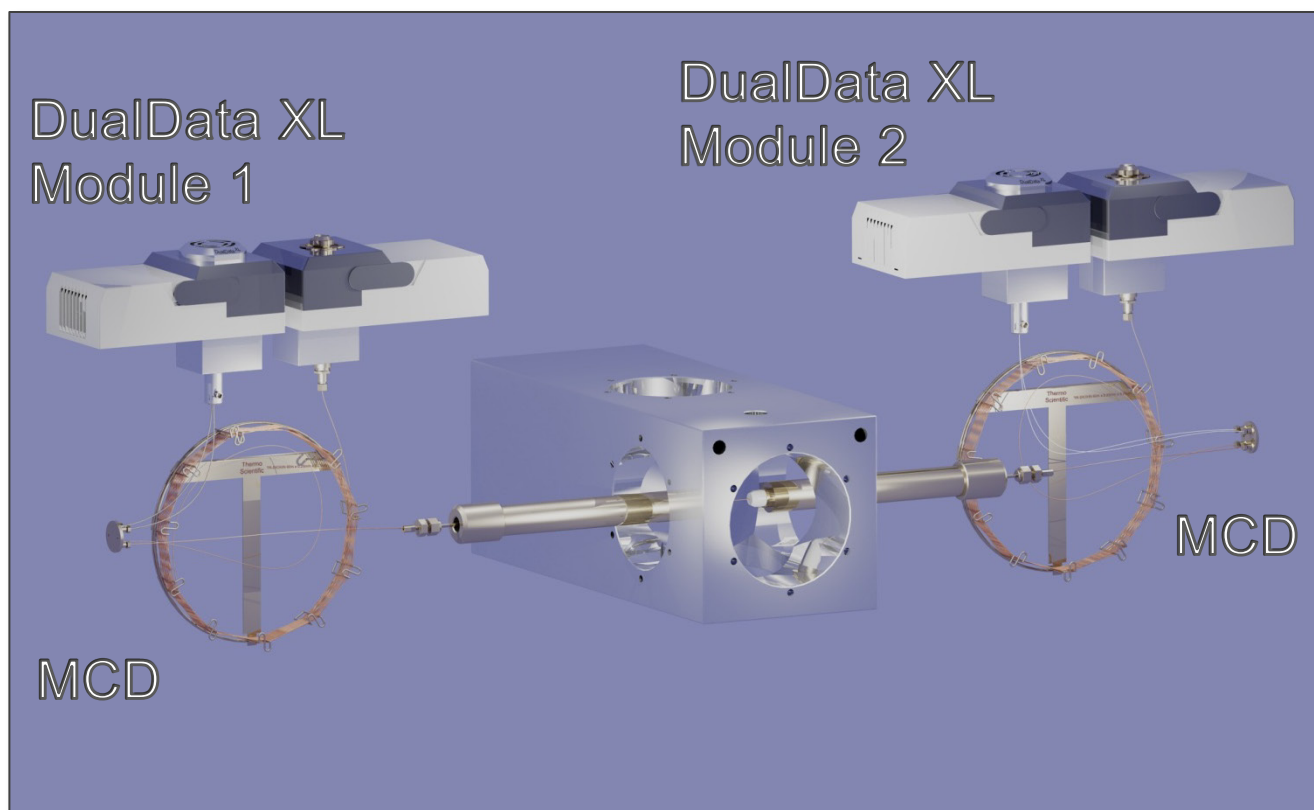
Hardware: DFS Magnetic Sector GC-HRMS with 2 Trace 1310 GC & 1 RSH Autosampler

- Standard Dual GC DFS

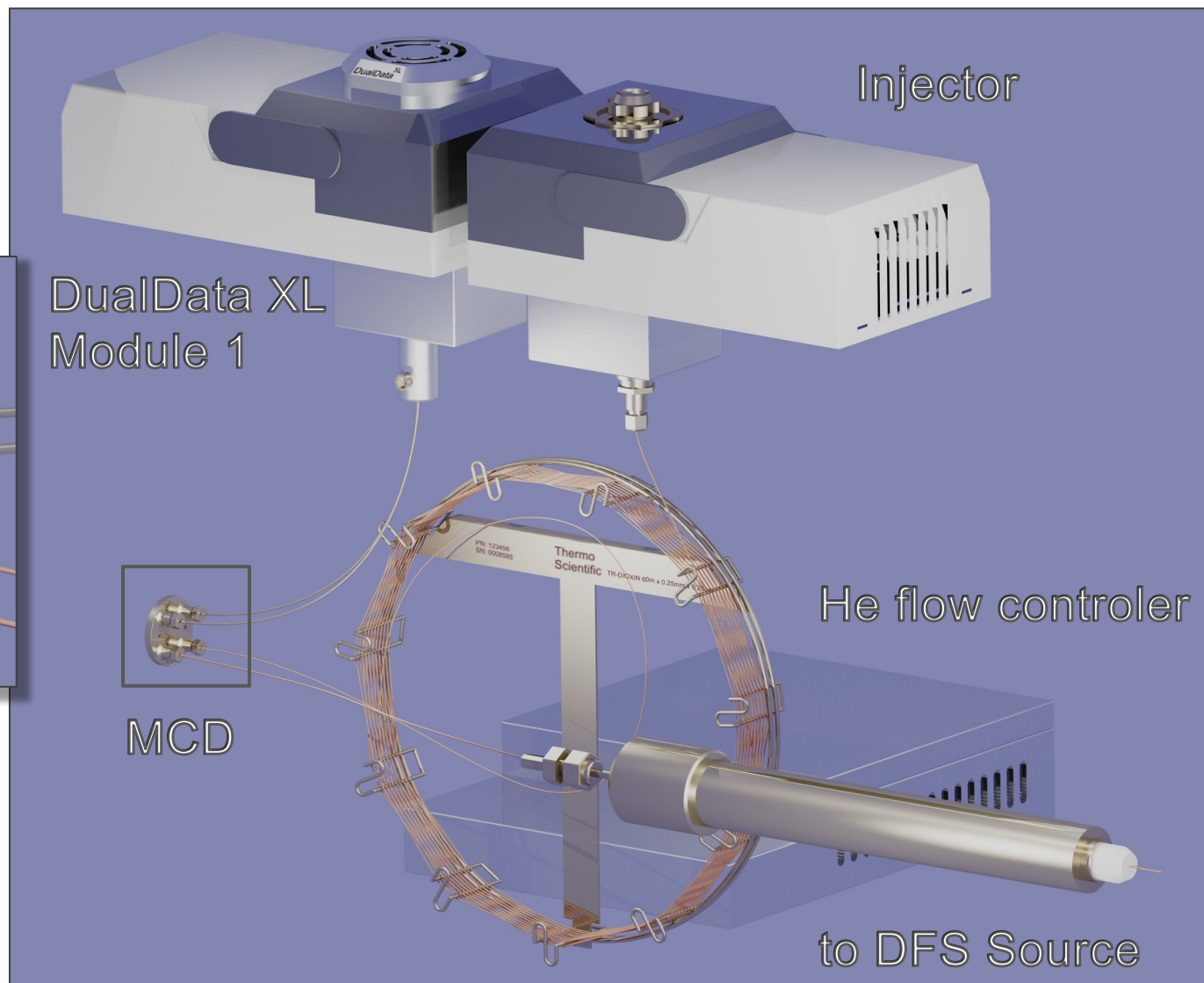


Hardware: DualData XL modules & MCD in each GC

- DFS Magnetic Sector GC-HRMS DualData XL GC-HRMS



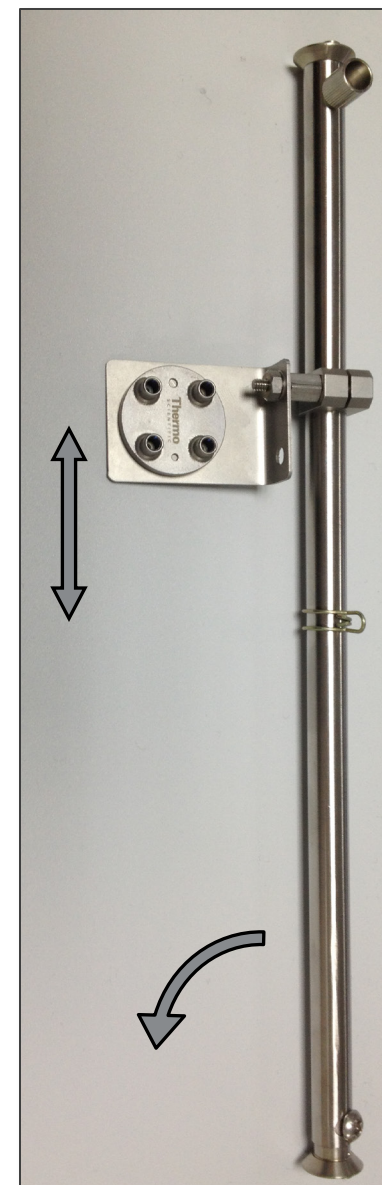
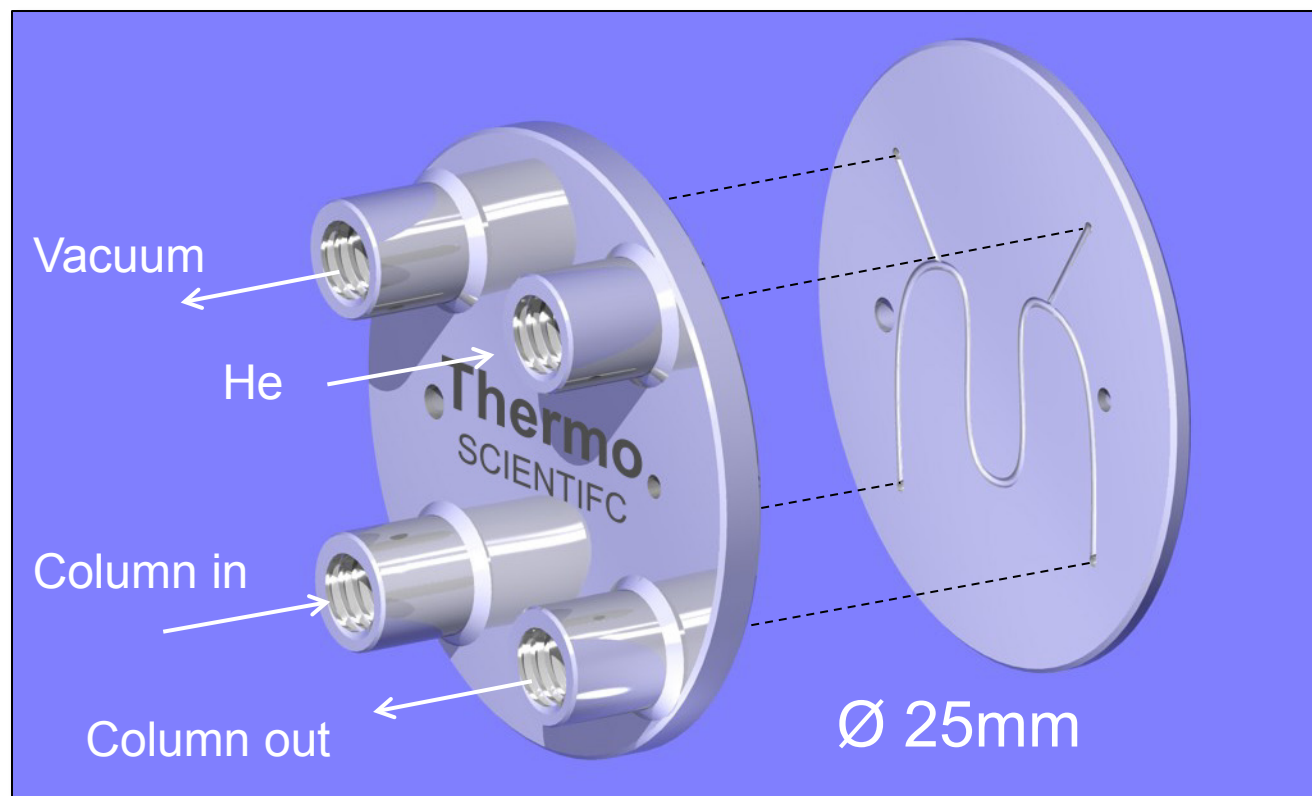
Hardware: DualData XL modules, MCD & Carrier Gas module



MCD:
Multi channel Device

DFS DualData XL: Micro Chanel Device Wafer

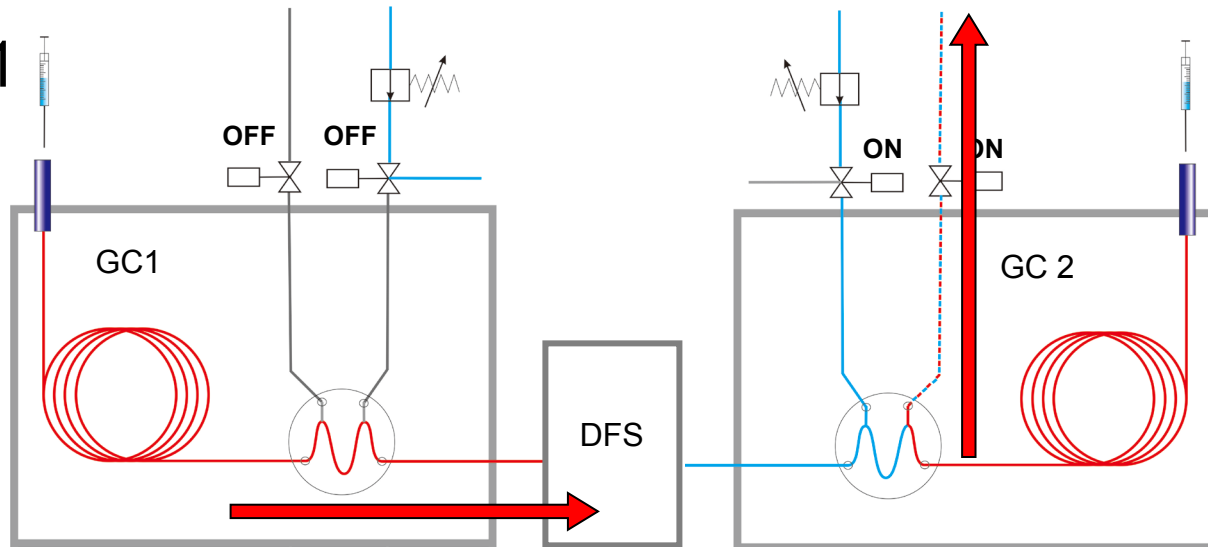
- Easy installation of capillaries
- Completely leaktight
- No deadvolume, perfect peakshapes
- Additional benefit: change column without venting DFS Source.



Alternating Flow switching with both GCs

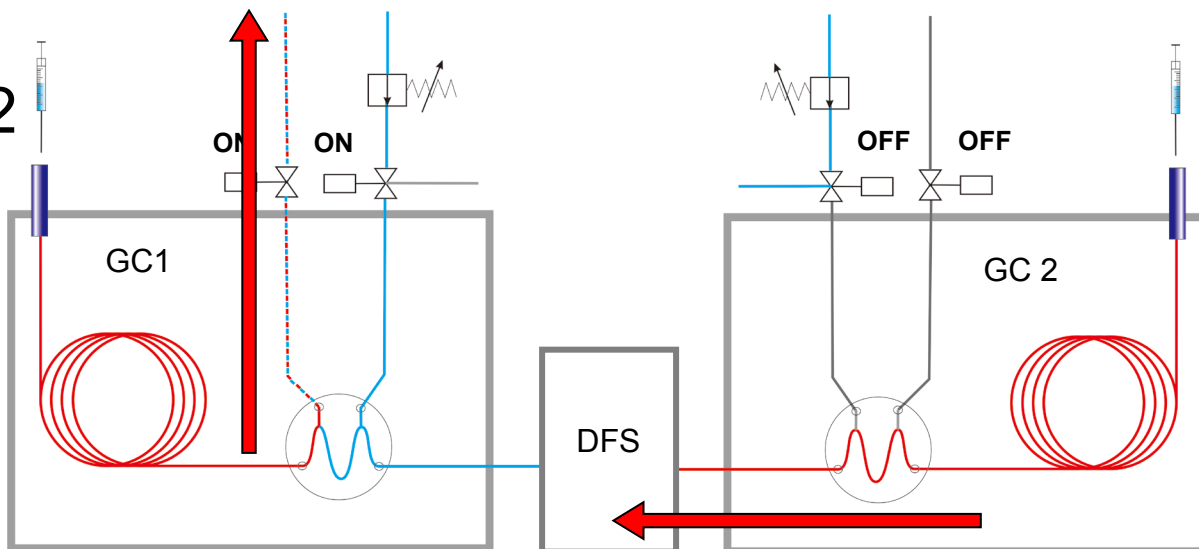
- **A: Acquisition GC1**

- GC1 into MS
- GC2 into waste



- **B: Acquisition GC2**

- GC2 into MS
- GC1 into waste



DFS DualData XL Software

- DualData XL = 2 x GC-HRMS Systems (2 Devices)
- Each device with with individual GC, Autosampler and MS settings.

The screenshot displays the DFS DualData XL software interface, which is divided into several functional areas:

- Config Files:**
 - GC 1:** Mode: MID-Method, Method: Dioxin_MID_GC1.mid, MID Path: C:\Xcalibur\System\DFS\Msi\Dioxin_MID_GC1.mid
 - GC 2:** Method: Dioxin_MID_GC2.mid, MID Path: C:\Xcalibur\System\DFS\Msi\Dioxin_MID_GC2.mid
- Chromatograms:**
 - A main chromatogram showing peaks at retention times: 21.63, 22.40, 22.80, 24.64, 25.53, 26.40, 27.47, 28.55, 29.44, 29.89, 30.20, 31.51, 33.48, 35.08, 36.08, 37.95, 39.48, 39.92, and 40.67 minutes.
 - A zoomed-in view of the 36-42 minute range, highlighting peaks at 36.08, 37.95, 39.48, and 39.92 minutes.
- MID Settings:**
 - Method: Dioxin_MID_GC2_FC43.mid
 - Segments: 6
 - Acquire Time [min]: 42.00
 - MID Mode: Lock
 - Data Type: Centroid
 - Width 1st Lock [amu]: 0.20
 - Sweep Peak Width: 3.00
 - Offset [µV]: 20
 - Measure/Lock Ratio: 1
 - Magnetic Delay [ms]: 60
 - Electric Delay [ms]: 8
 - Dual Data Offset [min]: 21.00
- Segment Settings:**
 - Start [min]: 21.00, End [min]: 25.02, Measure [min]: 4.02, Cycle [sec]: 2.00
- Table:**

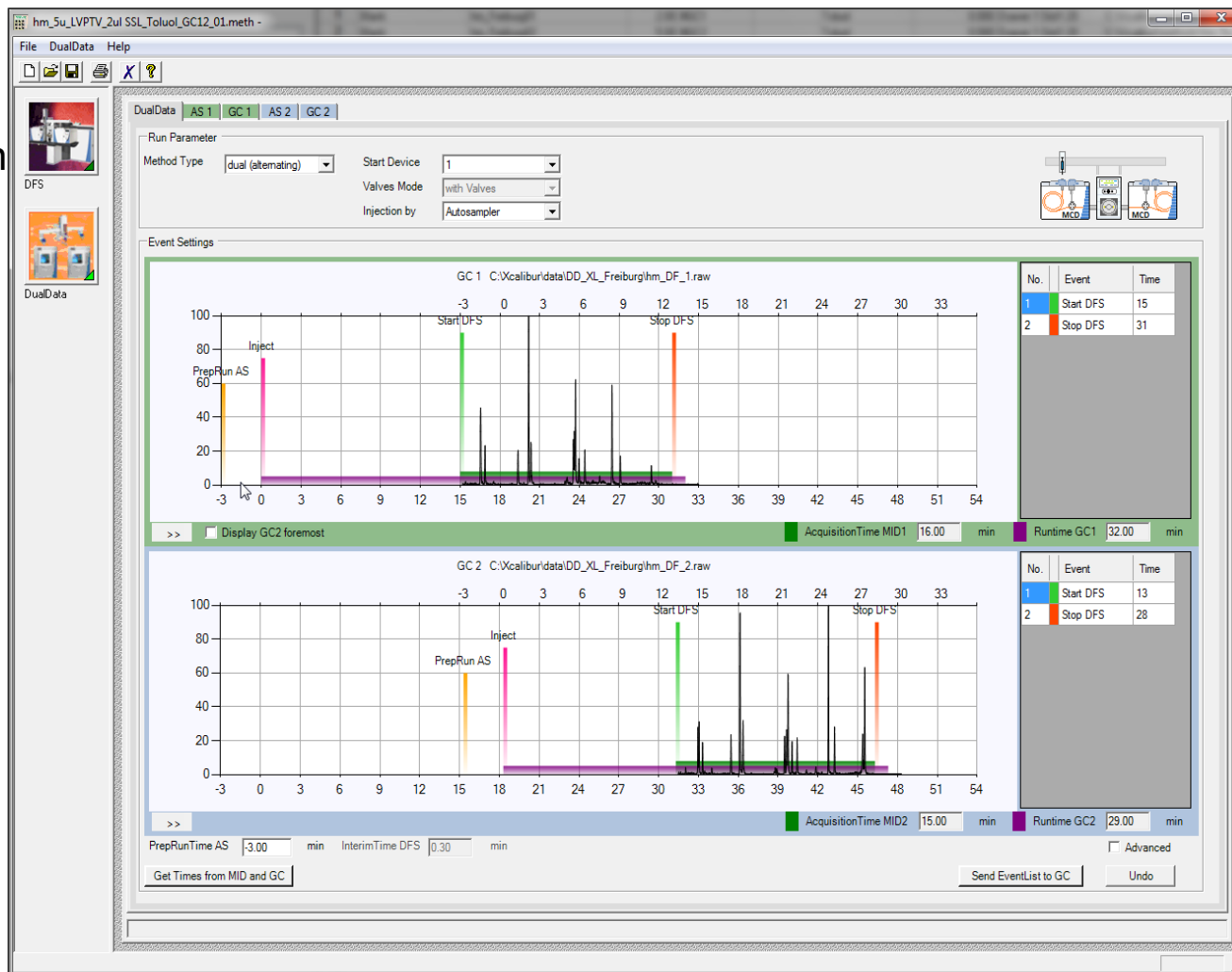
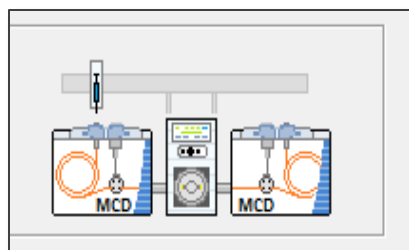
Section	L/C	Mass	Gr.	Int.	Time[ms]	Compound	Comment
1		303.90108	1	1	254	tdcf	RM native tdcf
2		305.89813	1	1	254	tdcf	QM native tdcf
3	Lock	313.98336	1	20	12	FC43	
4		315.94133	1	5	50	TCDF	RM [13]C- TCDF
5		317.93838	1	5	50	TCDF	QM [13]C- TCDF
6		319.89599	1	1	254	tdcd	RM native tdcd
7		321.89304	1	1	254	tdcd	QM native tdcd
8		331.93625	1	5	50	TCDD	RM [13]C TCDD
9		333.93330	1	5	50	TCDD	QM [13]C- TCDD
10		339.85915	1	1	254	pcdf	RM native pcdf
11		341.85620	1	1	254	pcdf	RM native pcdf
12		351.89941	1	5	50	PCDF	QM[13]C PCDF
13		353.89646	1	5	50	PCDF	RM [13]C PCDF
14	Calli	363.98017	1	20	12	FC43	
15		0.00000	0	0	0		RM [13]C PCDF
16		0.00000	0	0	0		RM [13]C PCDF

DFS DualData XL Software: Workflow

- Automatically calculation of all timing events based on MS and GC method.

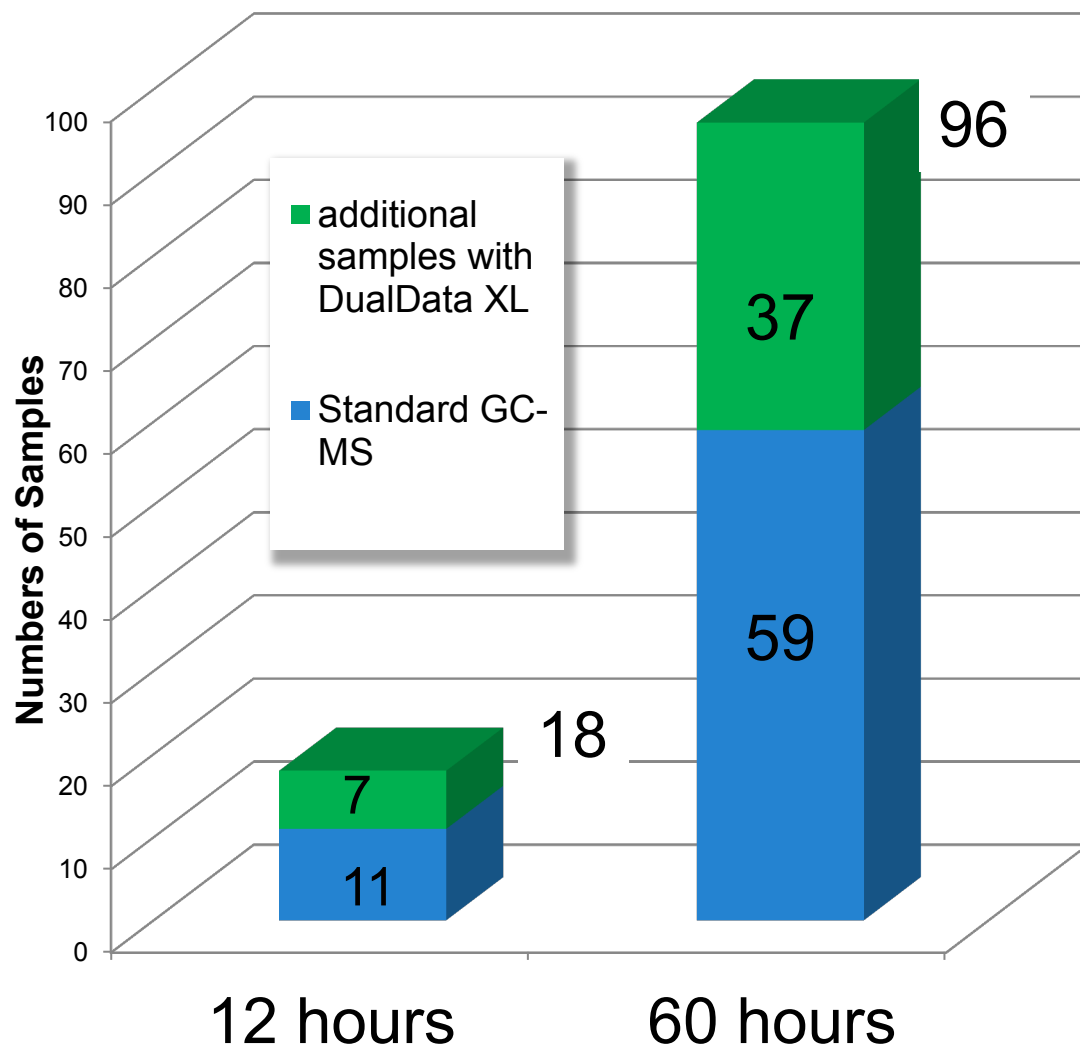
- Example:

- Staggered Injection
- Starting GC1



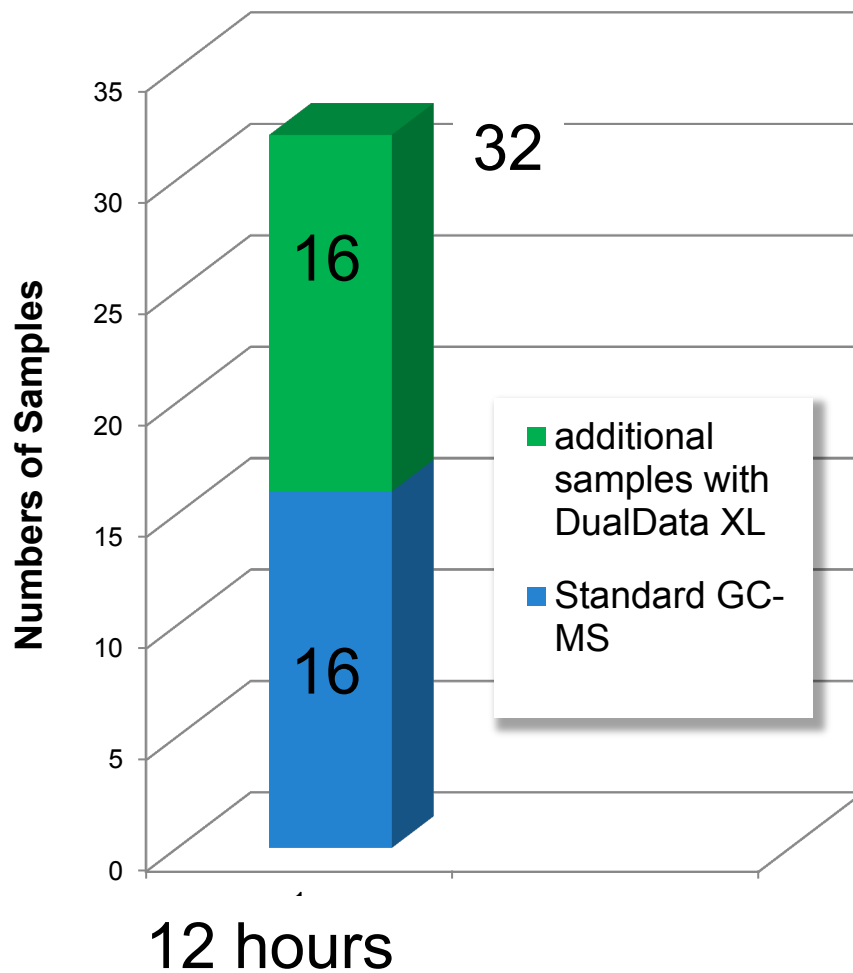
Beta Tester results: DFS DualData XL method

- With the standard method of the Lab:
- Increase in efficiency **63 %**
- Efficiency could be increased by further method optimization up to aprox. 88%



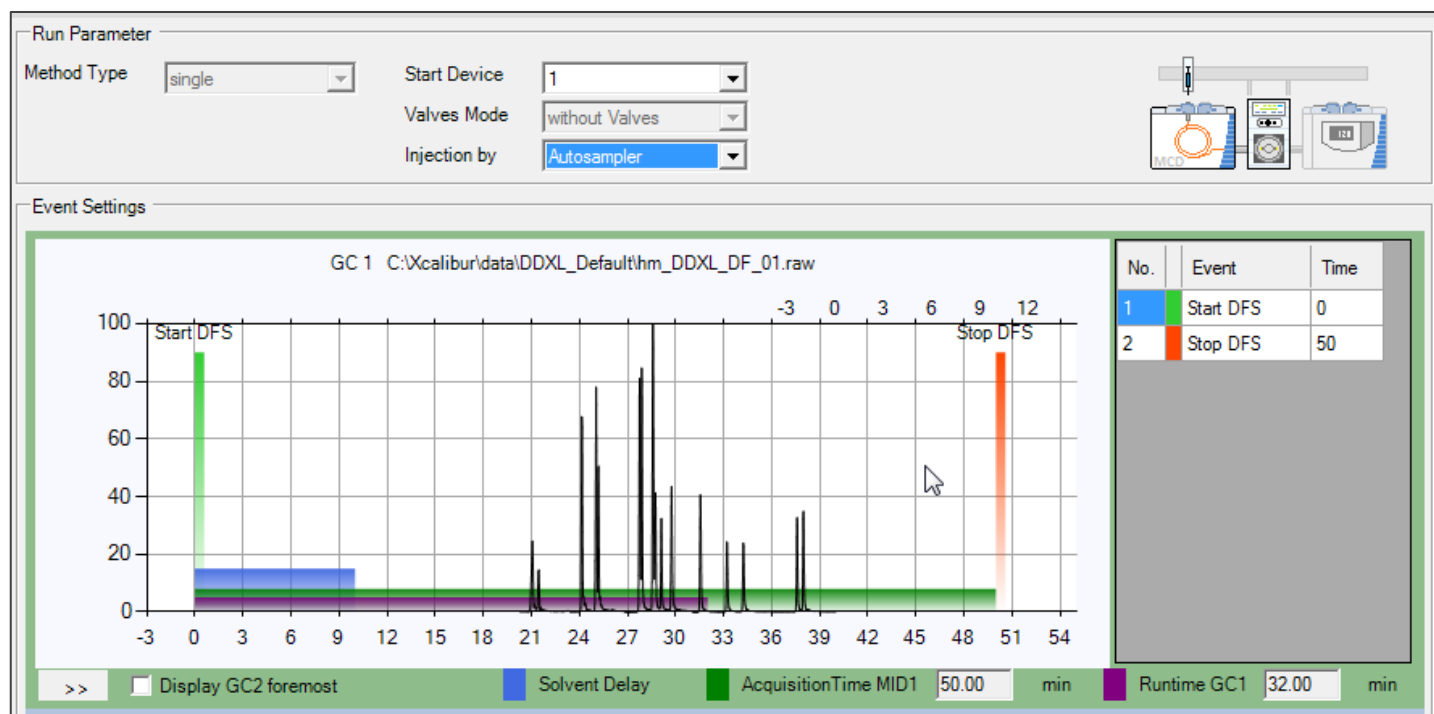
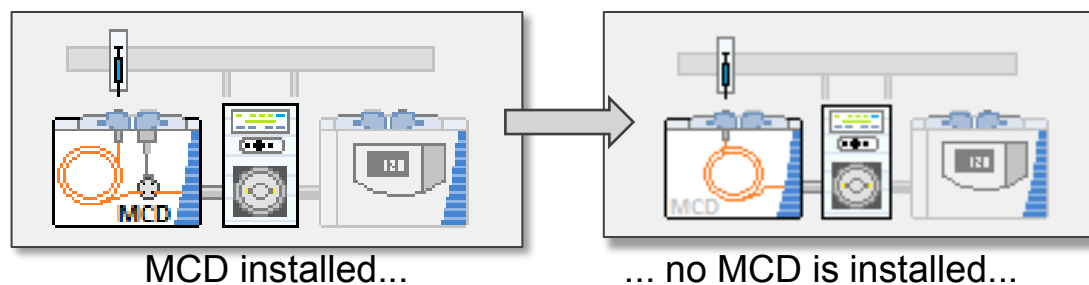
Time optimized method using DFS DualData XL

- Optimized method example:
 - **GC 1& GC 2:** GC = 43 min, MID =21 min
- Increase in efficiency aprox. **100%**



DFS DualData XL Software: Flexibility

- Example: no Hardware change necessary when no wafer is installed.
- GC column direct installed.

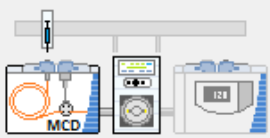


DFS DualData XL Software: Methods

- Create different experiments with a few clicks.

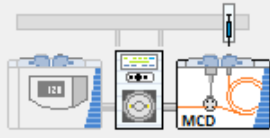
- Single method GC1

Run Parameter

Method Type	single	Start Device	1	
		Valves Mode	with Valves	
		Injection by	Autosampler	

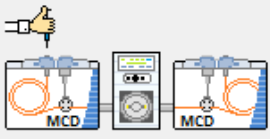
- Single method GC2

Run Parameter

Method Type	single	Start Device	2	
		Valves Mode	with Valves	
		Injection by	Autosampler	

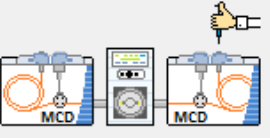
- Manually Injection GC1

Run Parameter

Method Type	dual (alternating)	Start Device	1	
		Valves Mode	with Valves	
		Injection by	manually	

- Manually Injection GC2

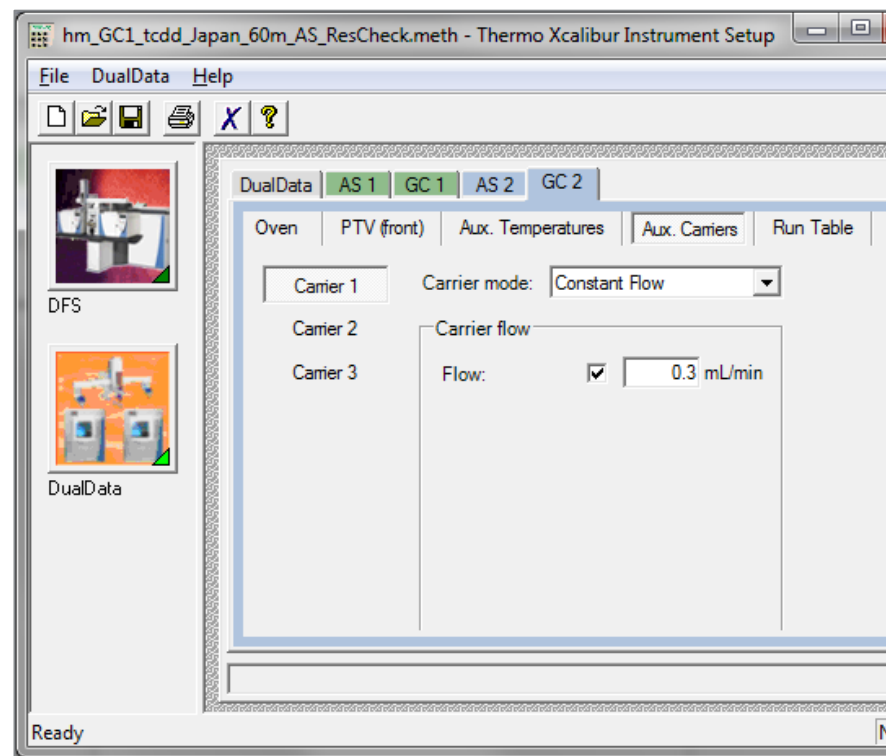
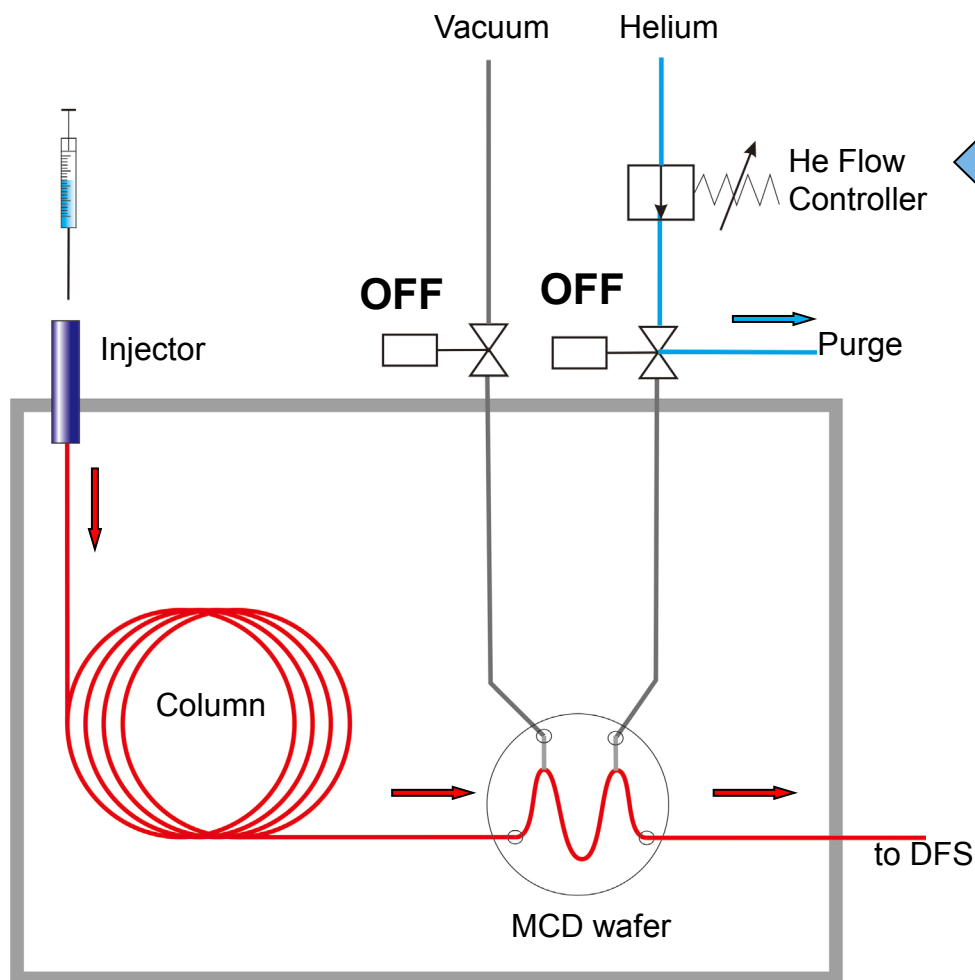
Run Parameter

Method Type	dual (alternating)	Start Device	2	
		Valves Mode	with Valves	
		Injection by	manually	

DualData XL Carrier Gas module

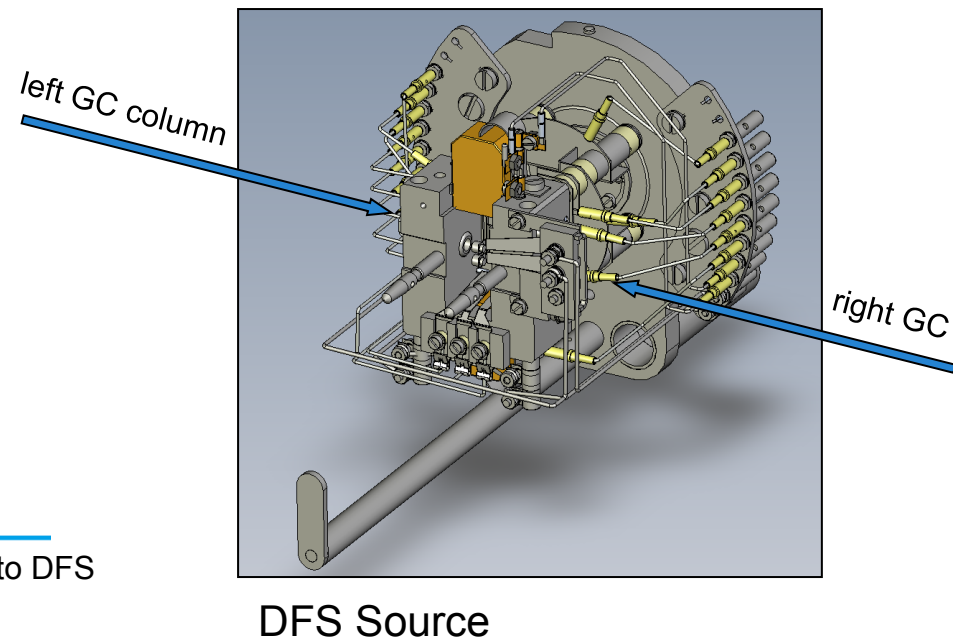
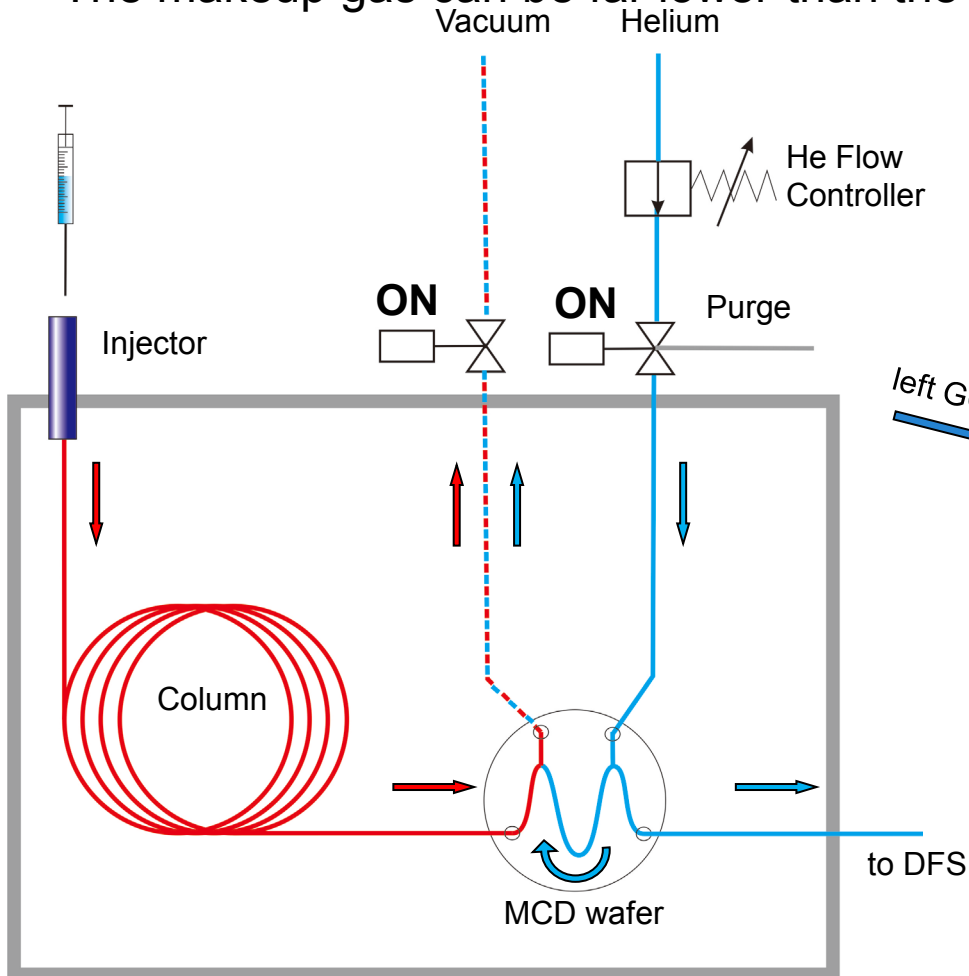


Hardware: Carrier Gas module



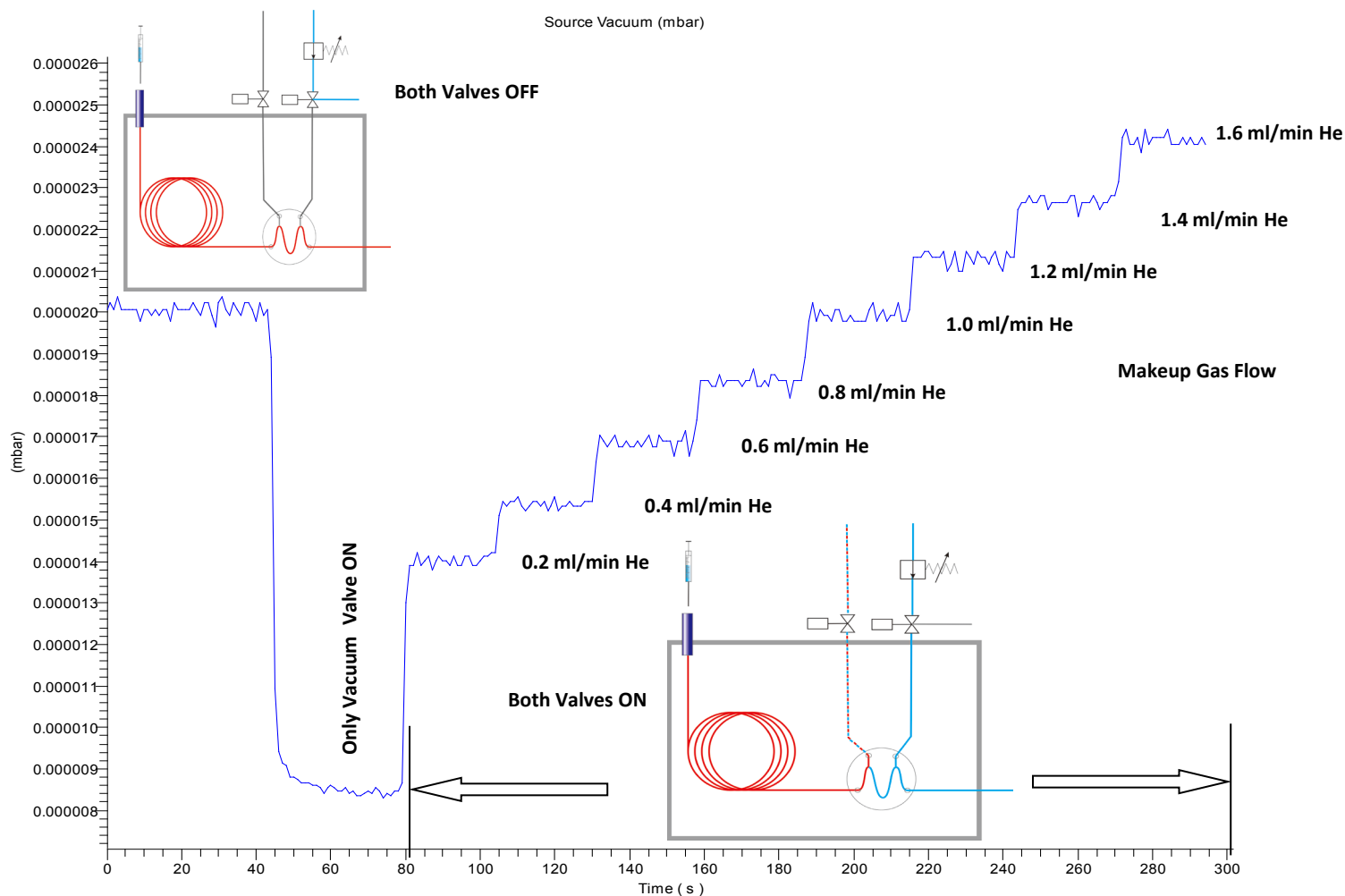
Hardware: Carrier Gas module

- Valves ON: the ion source pressure is independent from the column flow.
- It only depends on the makeup gas flow.
- The makeup gas can be far lower than the columnflow.



DFS DualData XL: Dynamic Flow Switching System

- **Ion source pressure with different valve position and makeup gas flows**



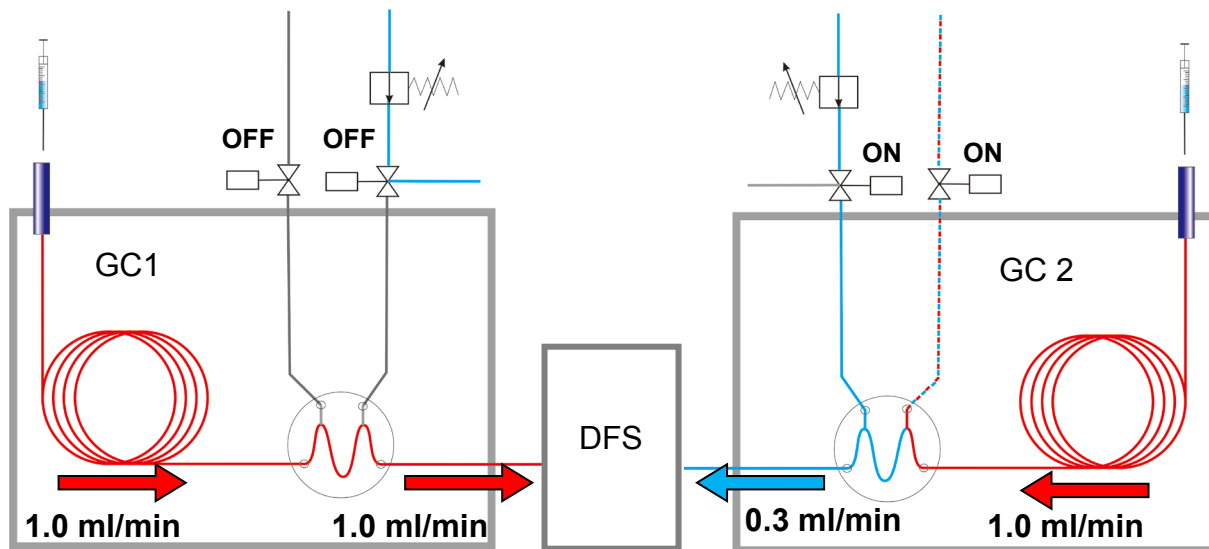
Ion source Pressure Profile with different gas flow rates delivered from the auxiliary gas module.

Alternating Flow switching with reduced Makeup Gasflow

- Within a sequence one column is always guided to the vacuum.
- The total flow load into the Ion Source is therefore makeup gas plus only one column flow.

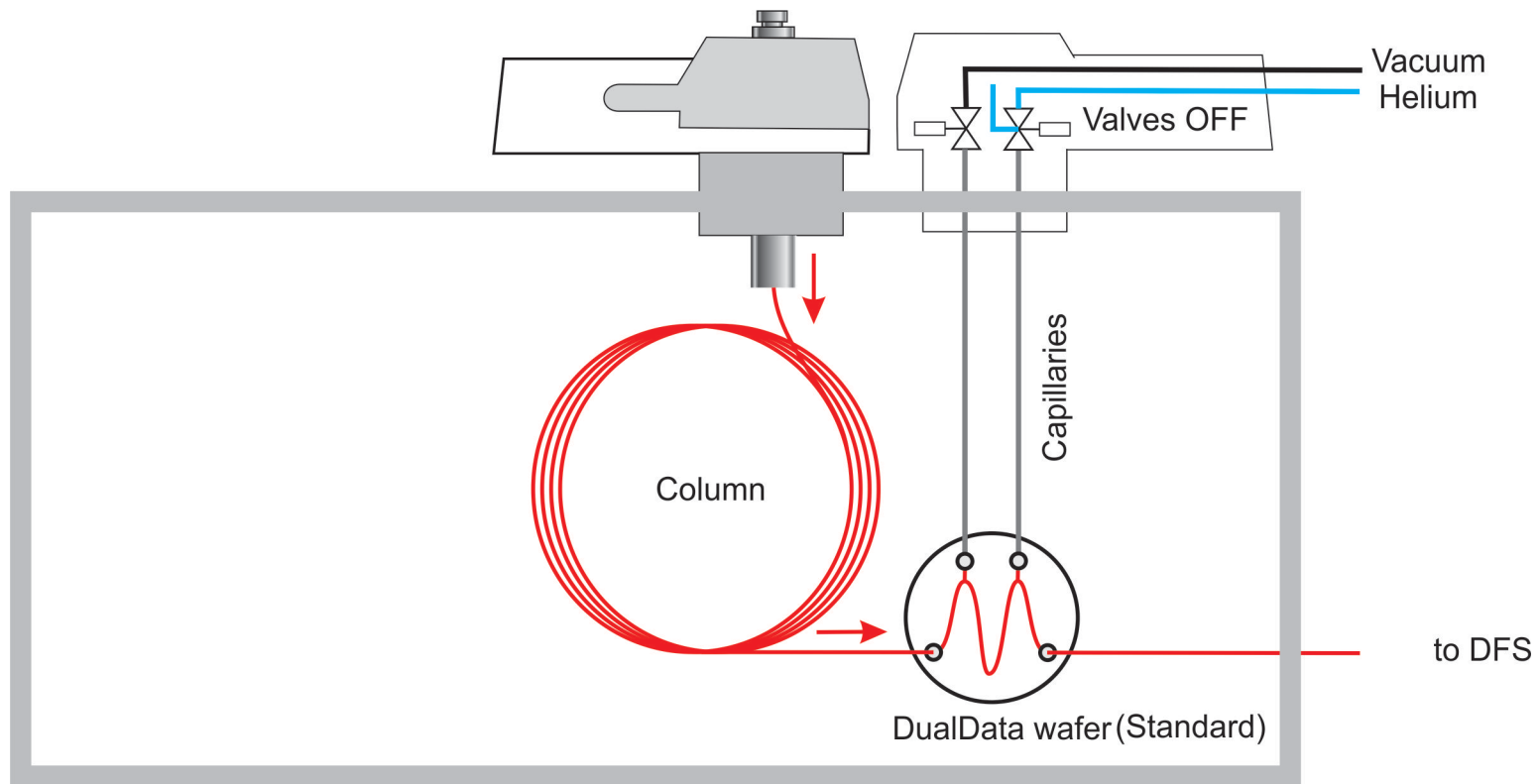
- **Example:**

- Column GC1: **1.0 ml/min**
- Column GC1: **1.0 ml/min**
- Makeup Flow: **0.3 ml/min**
- **He into DFS: 1.3 ml/min**

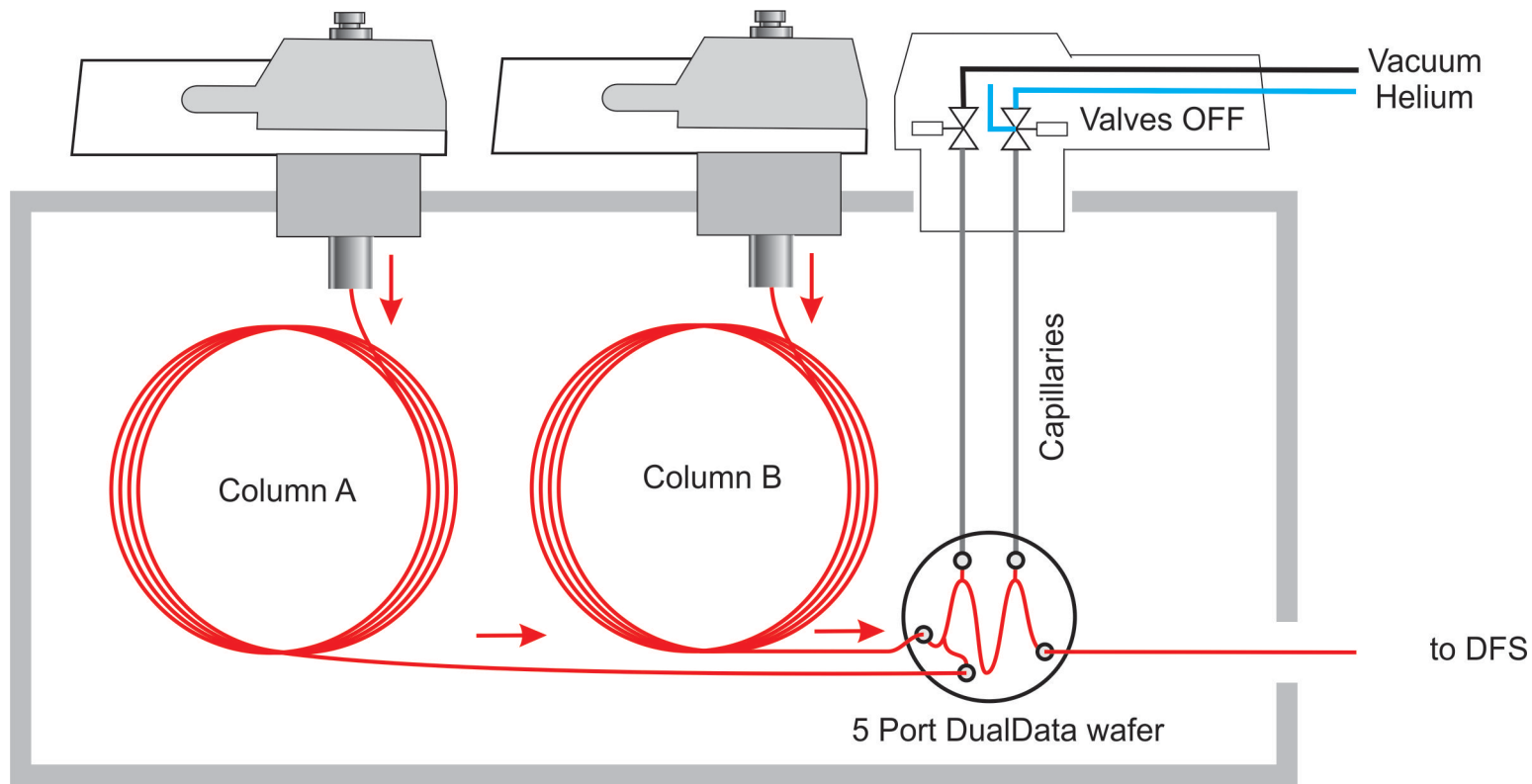


- It is also possible to run DualData with different column flows per GC.

DFS DualData XL: New Micro Chanel Device Wafer



DFS DualData XL: 5 Port Micro Channel Device Wafer



DFS DualData XL: 5 Port Micro Channel Device Wafer

- Setup Example using two 5 Port MCDs

	Injector	Column Type	Dimensions	
GC 1 Column A	SSL	DB5 MS	30m x 0.25mm 0.1um	PBDEs
GC 1 Column B	PTV	TR-PCB 8 MS	50m x 0.25mm 0.25um	PCBs
GC 2 Column A	PTV	VF5 MS	10m x 0.15mm 0.15um	BDE 209
GC 2 Column B	SSL	TR-Dioxin	60m x 0.25mm 0.25um	PCDD/F

DualData XL Conclusions

- Increase of sample throughput.
- Faster results
- Full Flexibility like standard dual GC DFS Magnetic Sector GC-HRMS.
 - Different Applications per GC (eg. GC1 Dioxin; GC2 BFRs etc.)
- Easy installation of capillaries
- Completely leaktight
- No deadvolume, perfect peakshapes
- MCD technology proven in routine.

- Additional benefit:
 - Fast change column without venting DFS Magnetic Sector GC-HRMS Source.
 - Condition one column while you measure on the other.
 - Less dirt into the Ion Source.

Discover the Gold Standard for Dioxin Analysis



Thermo Scientific DFS Magnetic Sector GC-HRMS