



Using Magnetic Sector DFS with DualData XL in a Commercial Dioxin Lab

- David Hope, P.Chem., CEO
- Pacific Rim Laboratories Inc.
- dave@pacificrimlabs.com

Overview

- History
- DualData – What is it?
- DualData XL – Why?
- DualData XL – Practical Applications
- Conclusions



Who Am I?

- Analytical Chemist
 - P.Chem. – ACPBC
 - Past-President, Canadian Council of Independent Laboratories
 - Owner, Lab Director, Quality Assurance Officer, Pacific Rim Laboratories
- I am not
 - Toxicologist
 - Consultant



PACIFIC RIM
LABORATORIES INC

My Business Partner and co-founder



- Patrick Pond
- Chief Technical Officer
- GC and HRMS instrument specialist



VG70 arrives!



Beginnings

Dioxin 2005 - Toronto



Thermo POPs Symposium– Venice 2007



More business means more instruments

First DFS (2007) – 1450 samples per year;
2250 tests – staff of 7

Second DFS (2010) – 2530 samples per year;
3500 tests – staff of 9

TSQ8000Evo (2014) – 3500 samples per year;
4450 tests – staff of 11

Third DFS (2015) – 4600 samples per year;
6750 tests – staff of 15

DualDataXL installed on DFS – projecting
6500 samples



PACIFIC RIM
LABORATORIES INC

Pacific Rim Laboratories Inc.

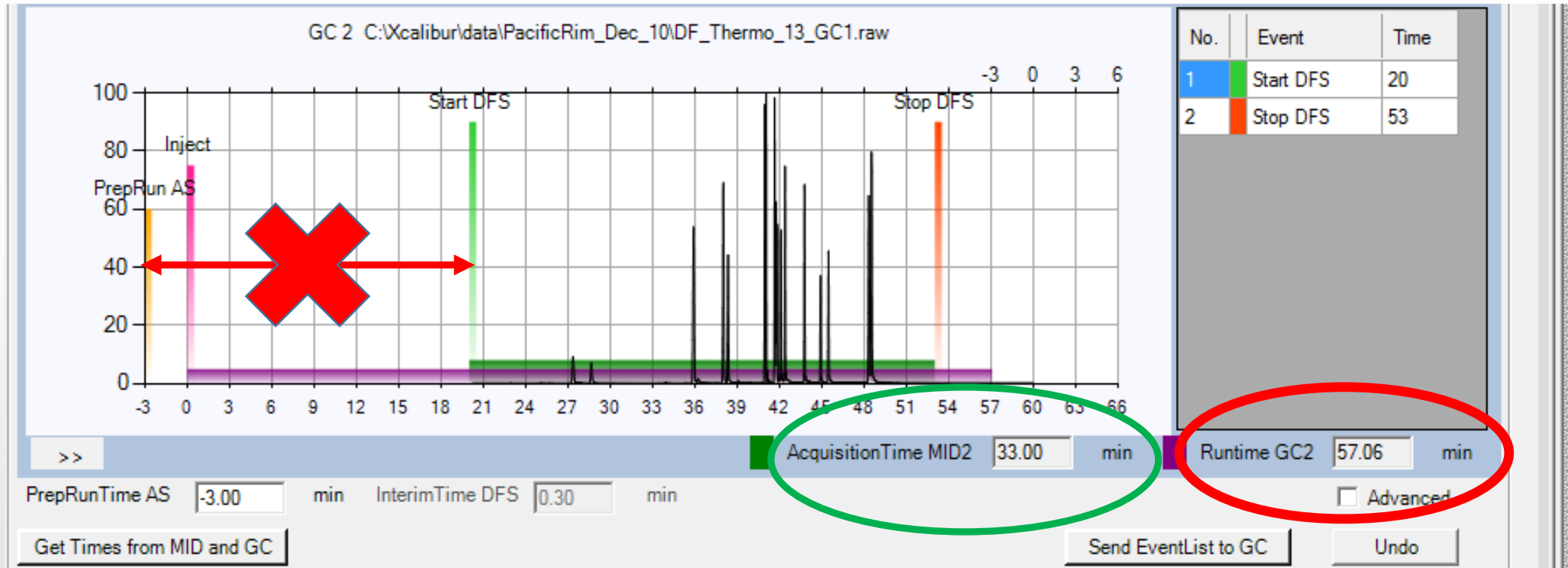
Scientific Research and Experimental Development

- We thrive on innovation
 - PBDE method in 2005
 - 209 congener PCBs in 2005
 - Sub-ppb PAH analysis food in 2006
 - Published 2009 congener PCB by SGE HT8 column (2009)
 - Cape Tech column clean-up (2012)
 - OCPs by HRMS (2012)
 - Improved clean-up methods for dioxins/PCB (2014)
 - Rocket evaporator (2015)
 - Single run PAH and alkylated PAH on TSQ8000Evo (2015)



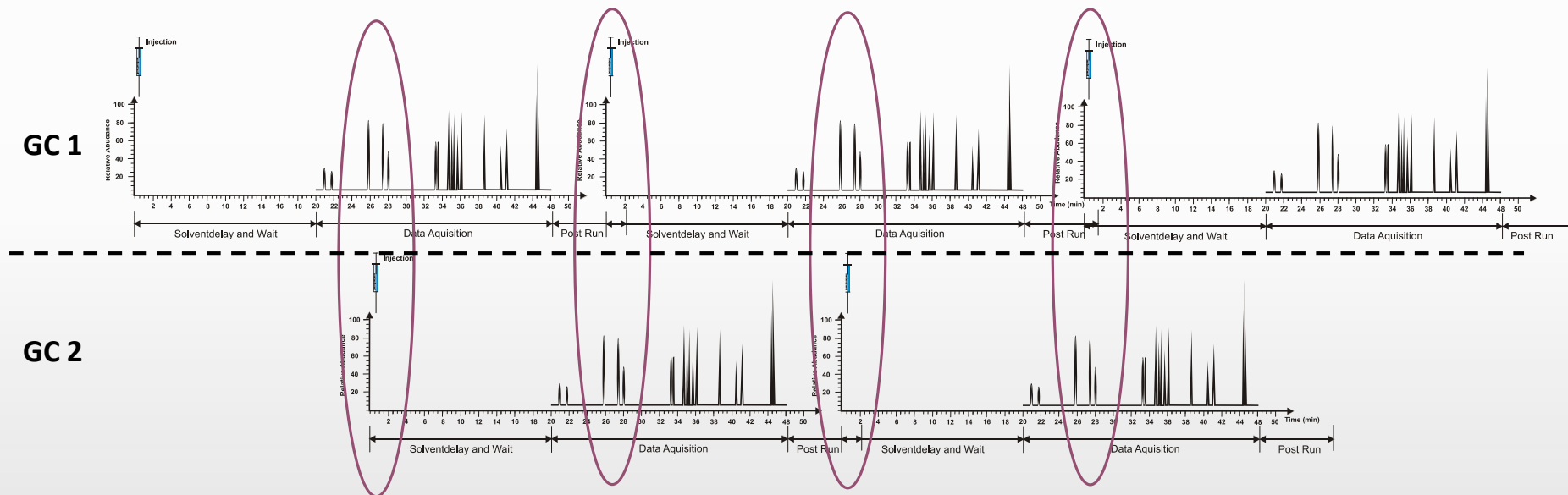
What is Dual Data? PCDD/F analysis

EPA 1613b – TCDD must elute >25 minutes



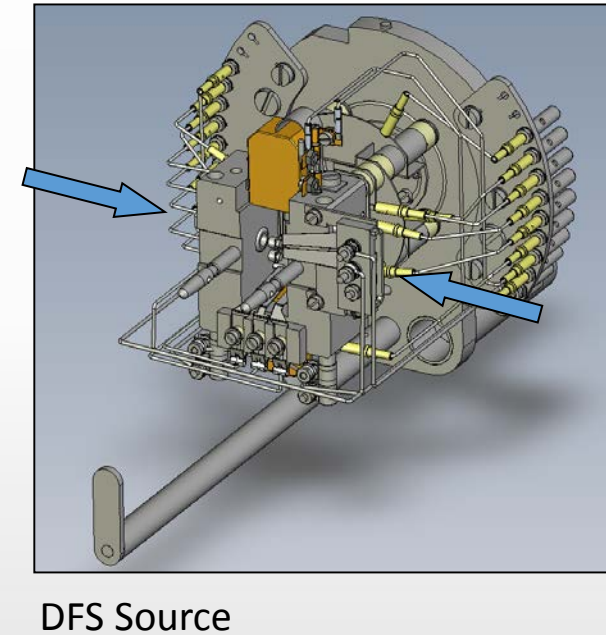
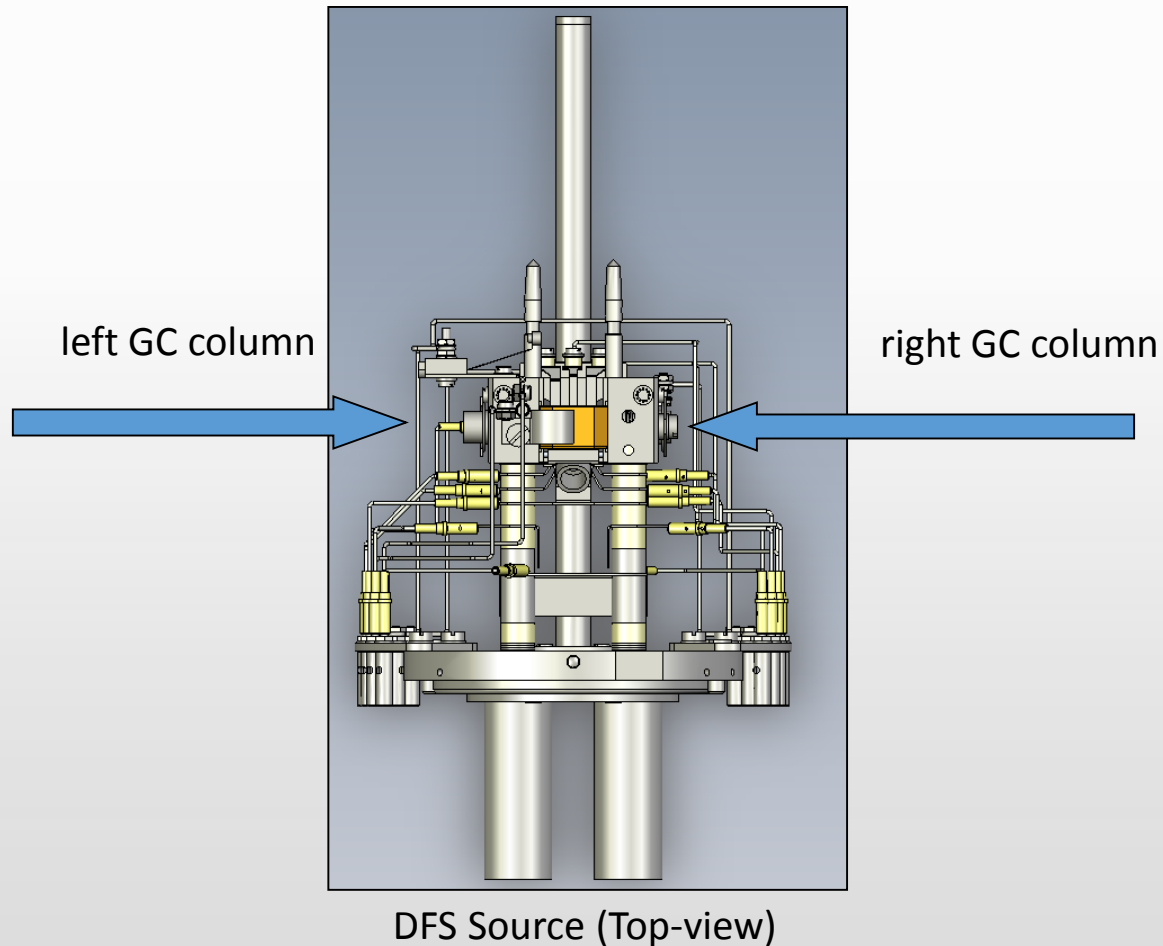
DFS DualData XL: Staggered Injection

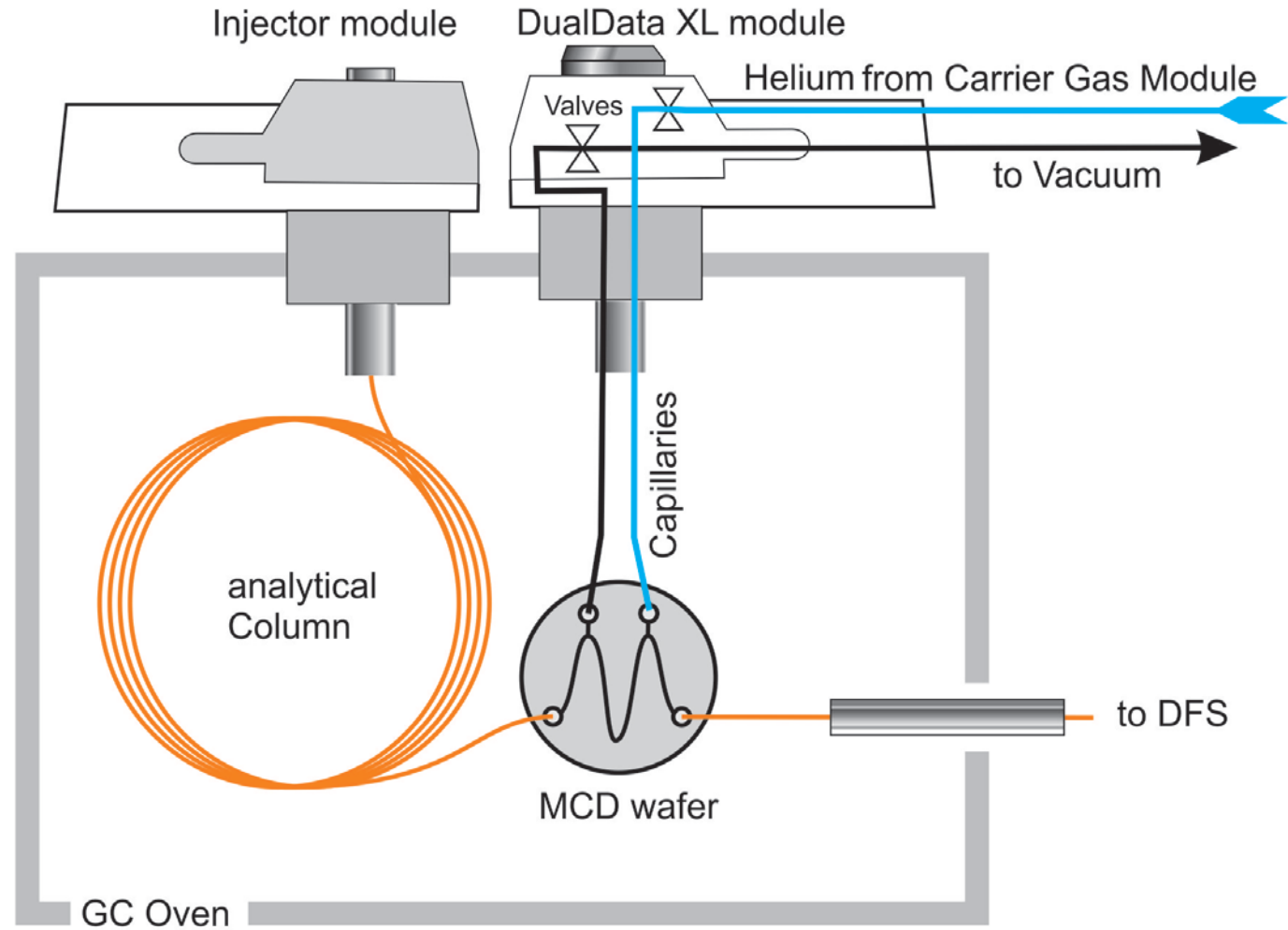
- Both GCs are running simultaneously.
- The injection on GC 2 is performed during the acquisition of GC 1 and vice versa.



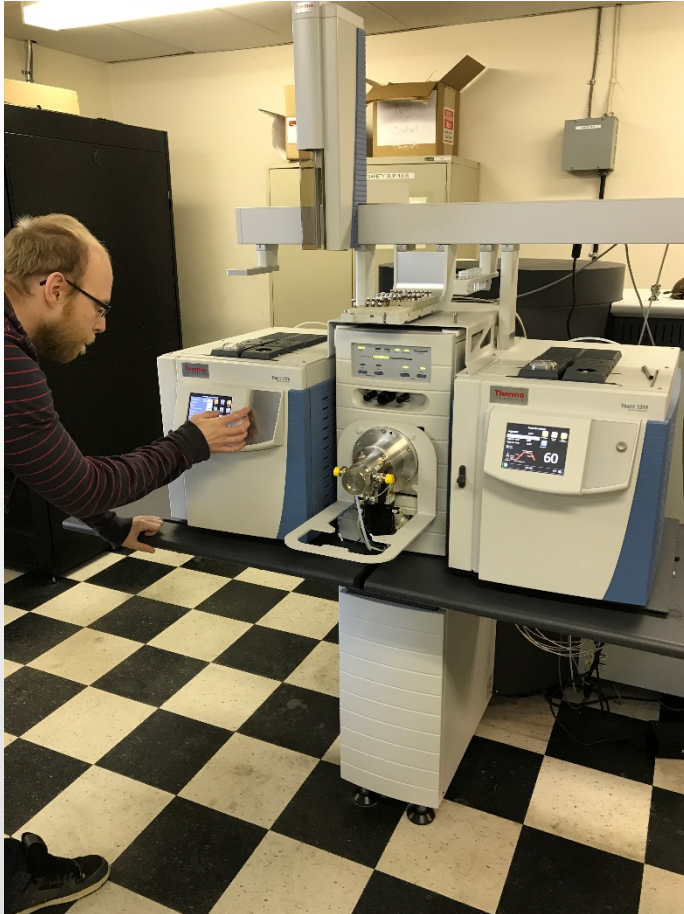
Columns from both GCs attached to one DFS Ion source

- Both columns are directed into the source





Why DualData XL?



- Cheaper than buying new instrument
- No additional floor space required
- No additional electrical considerations
- Autosampler ready to inject as soon as we get ready signal
- Can double our through put with mixed chemistries



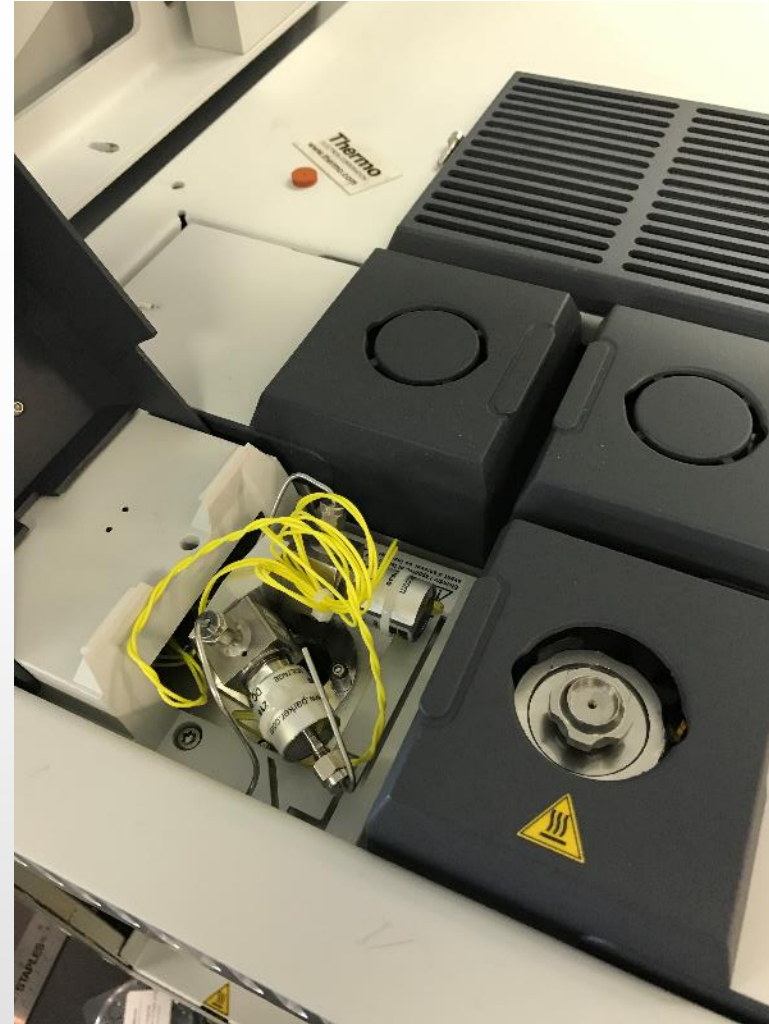
Requirements

- DFS with dual 1310 GCs
- Older DFS can be converted, but cannot use Trace GCs.
- Will add a 6-way valve to control gases



Requirements

- DFS with dual 1310 GCs
- Older DFS can be converted, but cannot use Trace GCs.
- Will add a 6-way valve to control gases
- A gas module is installed next to your injector.

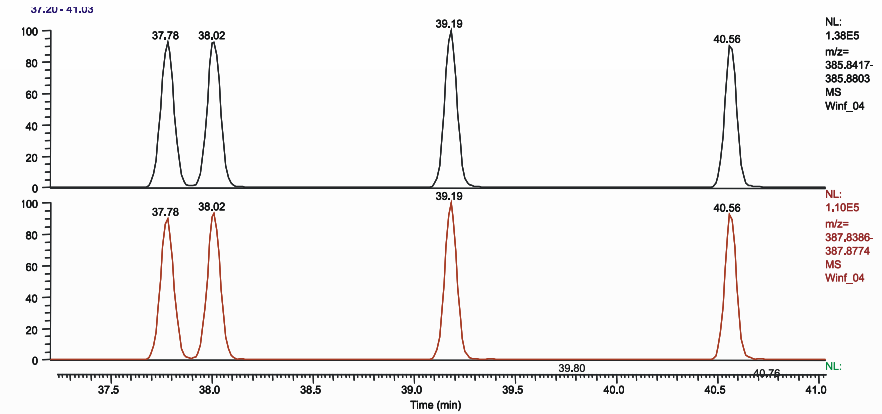
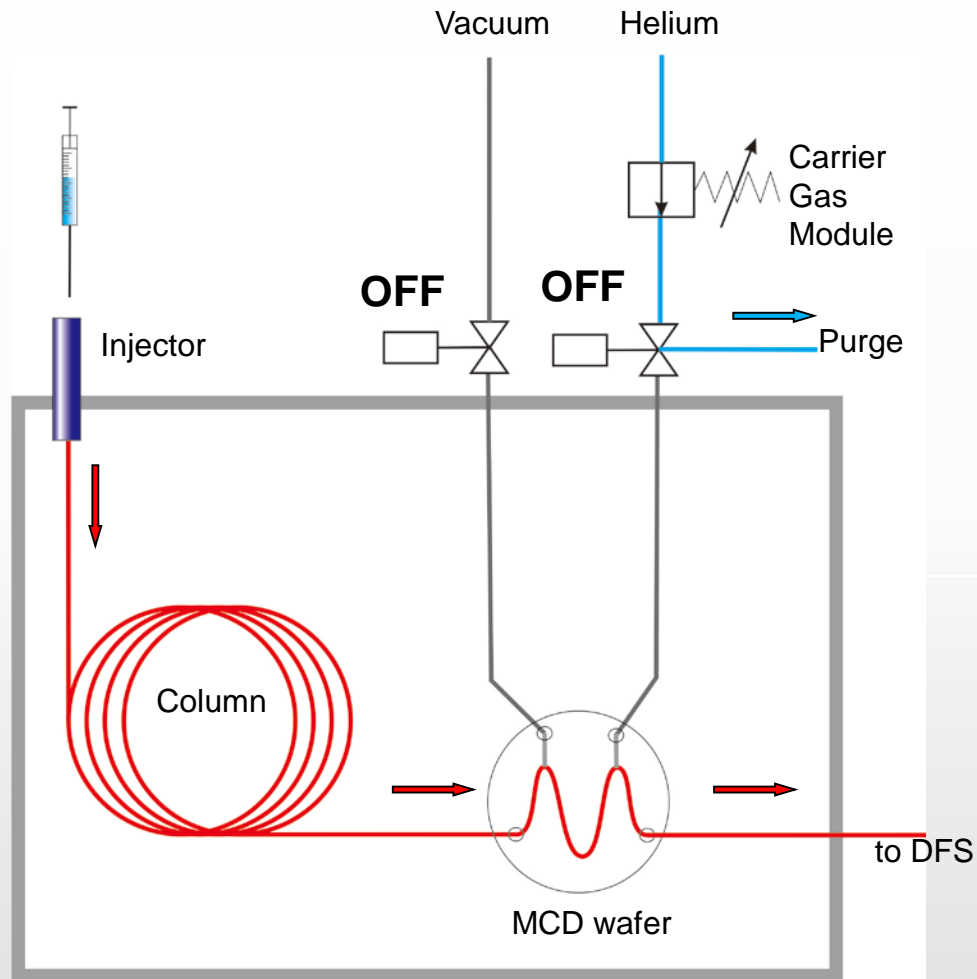


Requirements

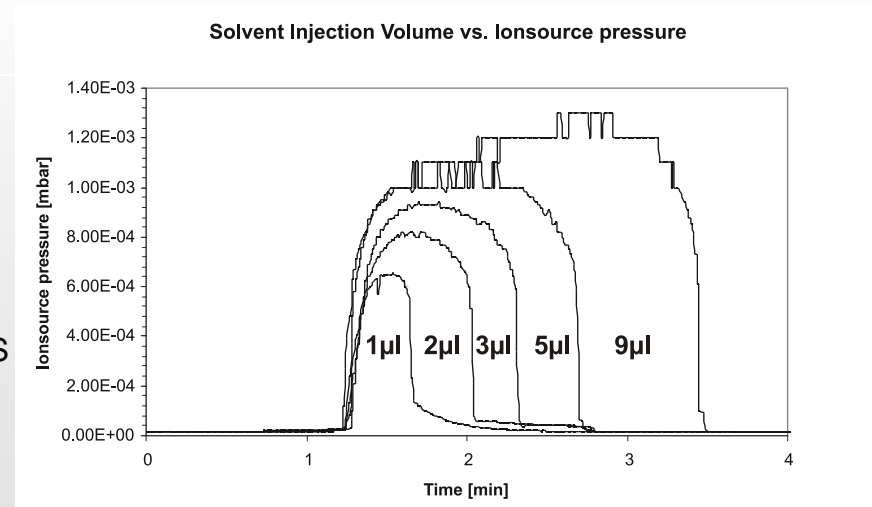
- DFS with dual 1310 GCs
- Older DFS can be converted, but cannot use Trace GCs.
- Will add a 6-way valve to control gases
- A gas module is installed next to your injector.
- New software



Flow switching 1: Column-flow is directed into the MS



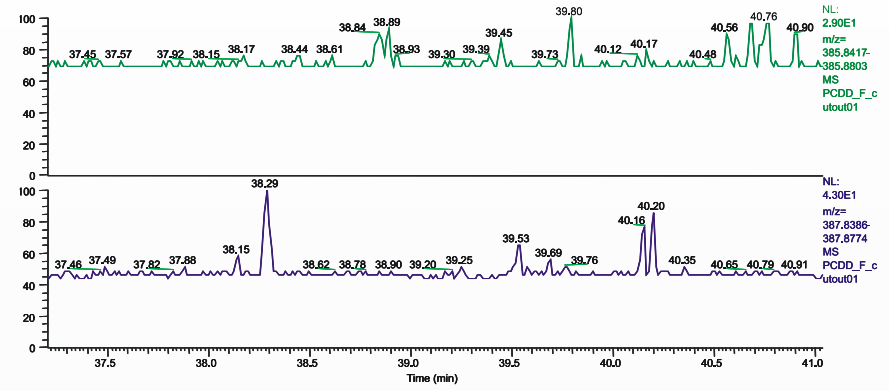
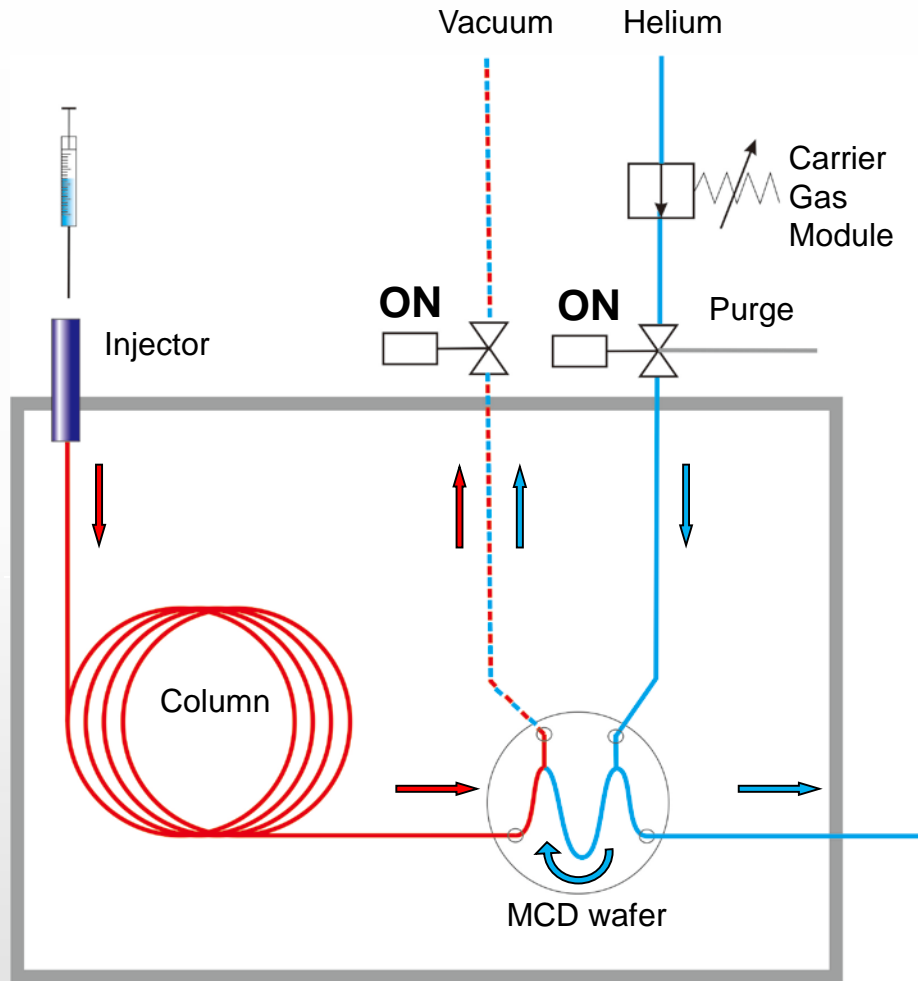
Example Standard inj.



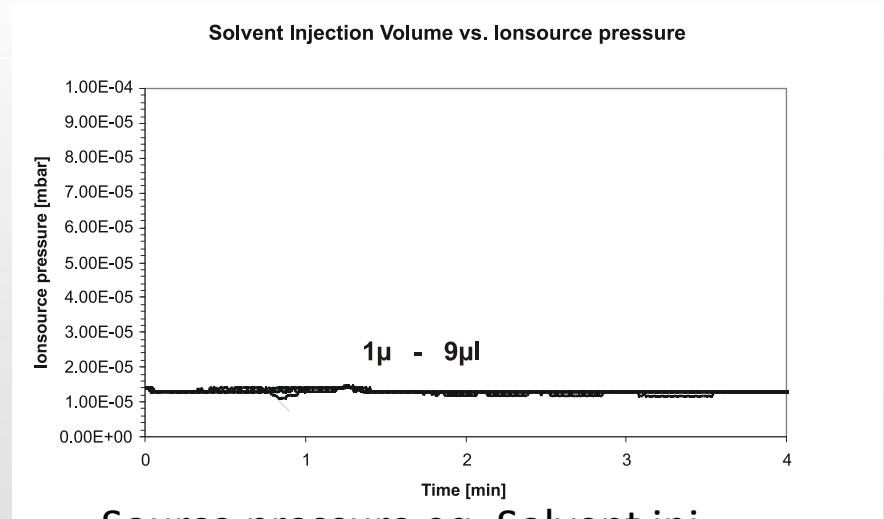
Source pressure eq. Solvent inj.



Flow switching 2: Flow directed into service vacuum (waste)



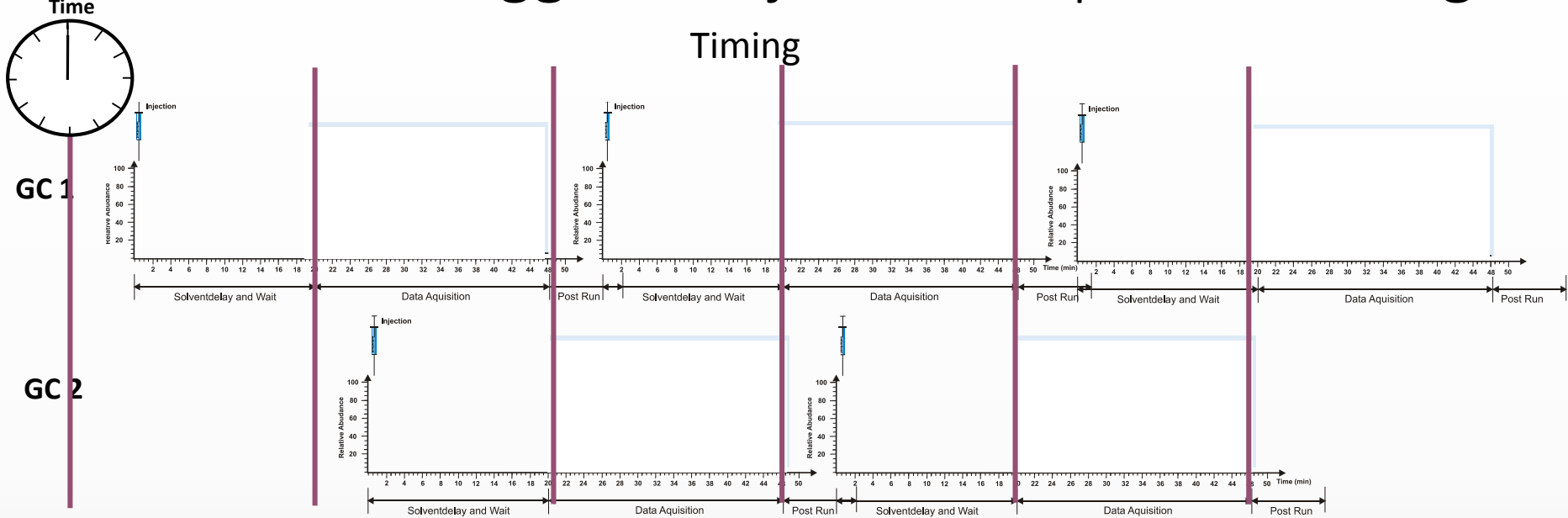
Example Standard inj.



Source pressure eq. Solvent inj.



DFS DualData XL: Staggered Injection Sequence Timing





*DFS



DualData

DFS

Config Files

GC 1

Mode: MID-Method | DDXL_WPCB_GC2_NEW.mid | Edit

MID: C:\Xcalibur\System\DFS\Msi\DDXL_WPCB_GC2_NEW.mid

GC 2

DDXL_GC1_DF_5W_FC43_GC2.mid | Edit

MID: C:\Xcalibur\System\DFS\Msi\DDXL_GC1_DF_5W_FC43_GC2.mid

Acquisition Times [min]

Use Solvent Delay only if no DualData wafer is installed | Solvent Delay: 0

Additional Action

Scripts: []

Select: [] +

Resolution Check

Activate

Report Reference []

Target Resolution 10000

Resolution Validation

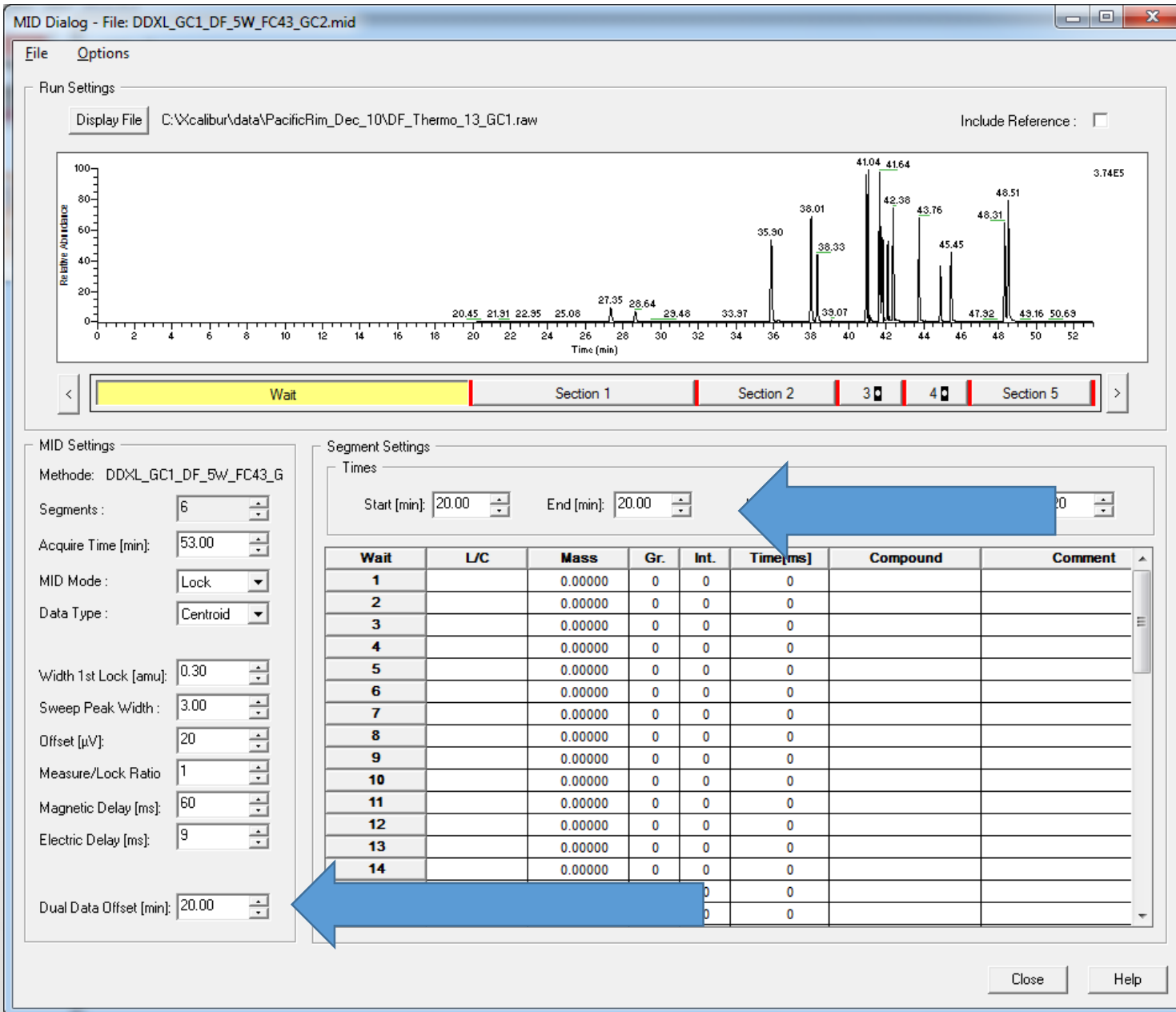
Warning if below 9500.00

Error if below 8000.00

Stop Sequence on Error

Lock Peak Mode: No Check





MID Dialog - File: DDXL_GC1_DF_5W_FC43_GC2.mid

File Options

- Advanced Scan Features
- DualDataMode

Run: ...Rim_Dec_10\DF_Thermo_13_GC1.raw Include Reference:

Chromatogram showing Relative Abundance vs Time (min). Peaks are labeled with retention times: 20.45, 21.91, 22.95, 25.08, 27.35, 28.64, 29.48, 33.97, 35.90, 38.01, 38.33, 39.07, 41.04, 41.64, 42.38, 43.76, 45.45, 47.32, 48.31, 48.51, 49.16, 50.63, and 3.74E5.

Wait Section 1 Section 2 3 4 Section 5

MID Settings

Method: DDXL_GC1_DF_5W_FC43_G

Segments: 6

Acquire Time [min]: 53.00

MID Mode: Lock

Data Type: Centroid

Width 1st Lock [amu]: 0.30

Sweep Peak Width: 3.00

Offset [µV]: 20

Measure/Lock Ratio: 1

Magnetic Delay [ms]: 60

Electric Delay [ms]: 9

Dual Data Offset [min]: 20.00

Segment Settings

Times

Start [min]: 20.00 End [min]: 20.00 Measure [min]: -0.00 Cycle [sec]: 0.20

Wait	L/C	Mass	Gr.	Int.	Time[ms]	Compound	Comment
1		0.00000	0	0	0		
2		0.00000	0	0	0		
3		0.00000	0	0	0		
4		0.00000	0	0	0		
5		0.00000	0	0	0		
6		0.00000	0	0	0		
7		0.00000	0	0	0		
8		0.00000	0	0	0		
9		0.00000	0	0	0		
10		0.00000	0	0	0		
11		0.00000	0	0	0		
12		0.00000	0	0	0		
13		0.00000	0	0	0		
14		0.00000	0	0	0		
15		0.00000	0	0	0		
16		0.00000	0	0	0		

Close Help



MID Dialog - File: DDXL_GC1_DF_5W_FC43_GC2.mid

MID Dialog - File: DDXL_GC1_DF_5W_FC43_GC2.mid

MID Dialog - File: DDXL_GC1_DF_5W_FC43_GC2.mid

MID Dialog - File: DDXL_GC1_DF_5W_FC43_GC2.mid

MID Dialog - File: DDXL_GC1_DF_5W_FC43_GC2.mid

File Options

Run Settings

Display File: C:\Xcalibur\data\PacificRim_Dec_10\DF_Thermo_13_GC1.raw

Include Reference:

Wait | Section 1 | Section 2 | 3 | 4 | Section 5

MID Settings

Method: DDXL_GC1_DF_5W_FC43_G

Segments: 6

Acquire Time [min]: 53.00

MID Mode: Lock

Data Type: Centroid

Width 1st Lock [amu]: 0.30

Sweep Peak Width: 3.00

Offset [µV]: 20

Measure/Lock Ratio: 1

Magnetic Delay [ms]: 60

Electric Delay [ms]: 9

Dual Data Offset [min]: 20.00

Segment Settings

Times

Start [min]: 46.50 End [min]: 53.00 Measure [min]: 6.50 Cycle [sec]: 0.80

Section 5	L/C	Mass	Gr.	Int.	Time[ms]	Compound	Comment
1		441.74280	1	1	134		
2		443.73980	1	1	134		
3		457.73710	1	1	134		
4		459.73770	1	1	134		
5	Lock	463.97378	1	10	13		
6		469.77800	1	3	44		
7		471.77500	1	3	44		
8	Call	501.97059	1	20	6		
9		513.67750	1	3	44		
10		0.00000	0	0	0		
11		0.00000	0	0	0		
12		0.00000	0	0	0		
13		0.00000	0	0	0		
14		0.00000	0	0	0		
15		0.00000	0	0	0		
16		0.00000	0	0	0		

Close Help



DDXL_WPCB_GC1_DF_GC2_WPCBONLY.meth - Thermo Xcalibur Instrument Setup

File DualData Help

DualData AS 1 GC 1 AS 2 GC 2

Run Parameter

Method Type: Start Device:

Valves Mode:

Injection by:

Event Settings

GC 1 C:\Xcalibur\data\PacificRim_Dec_10\DF_Thermo_22_GC1.raw

No.	Event	Time
-3	0	3
6	Start DEC	12

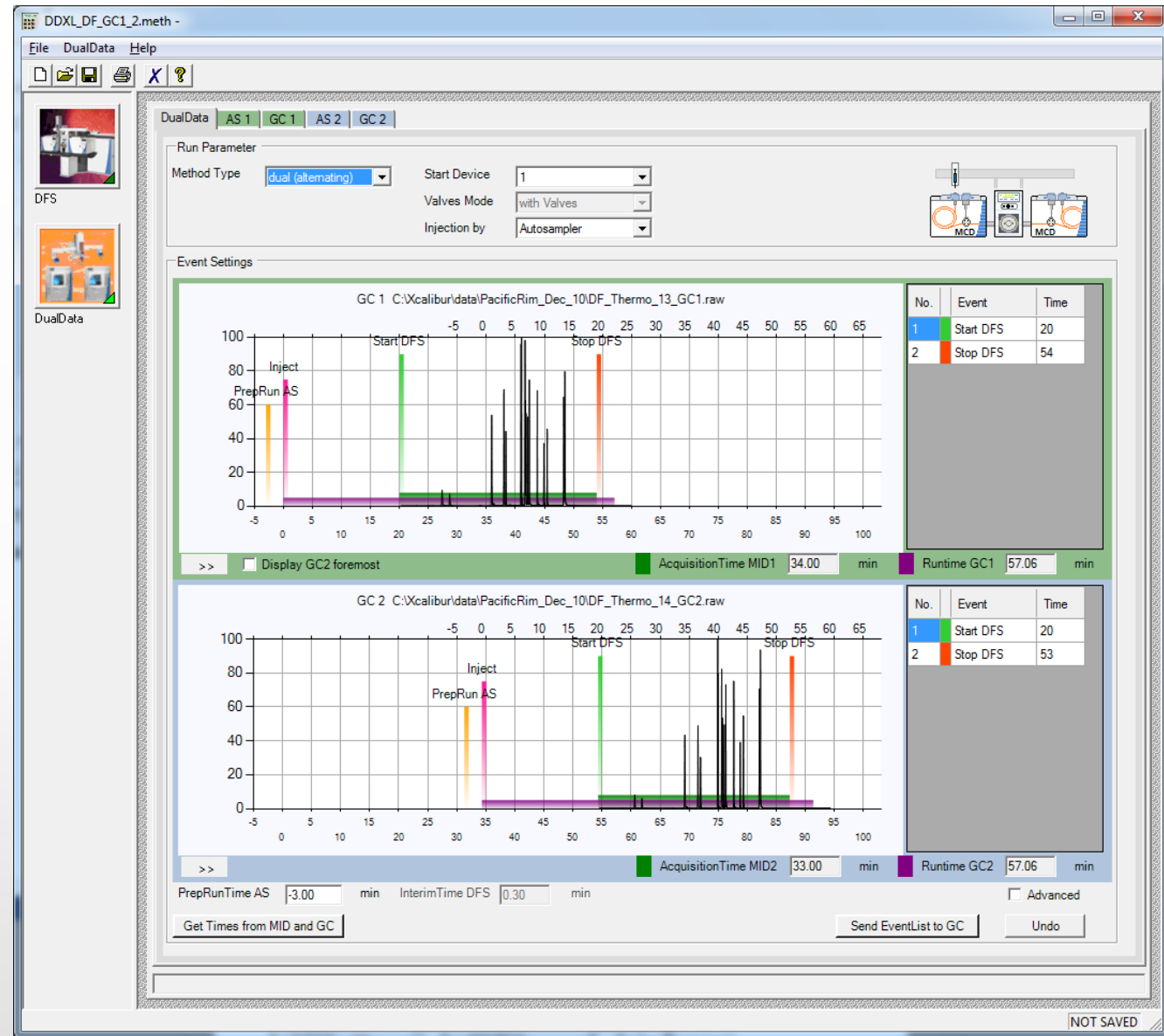


Dual PCDD/F

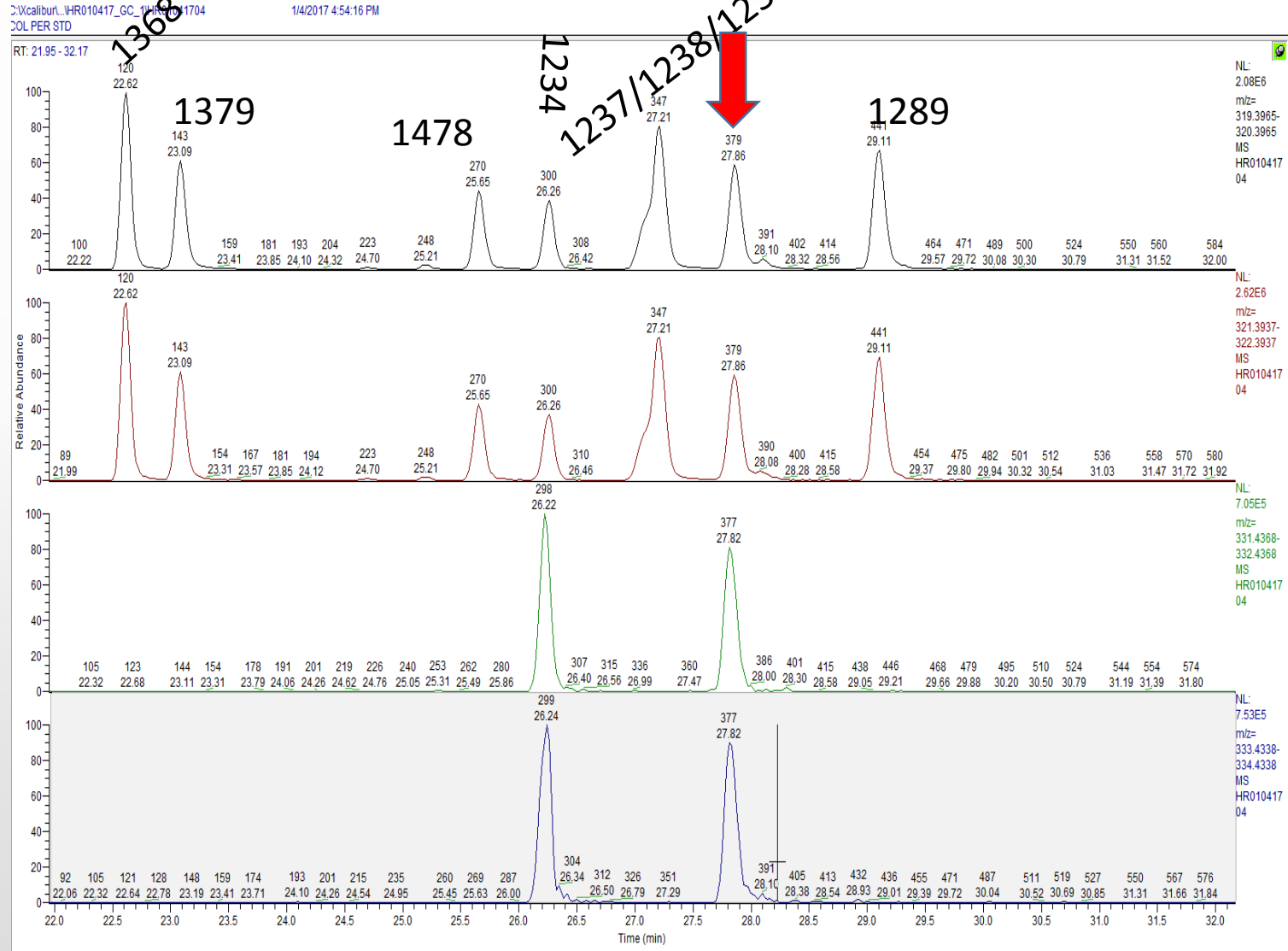
Runtime DFS – 62 minutes or 23 inj/day

Runtime DualData XL – 67 minutes or 42 injections in 24 h

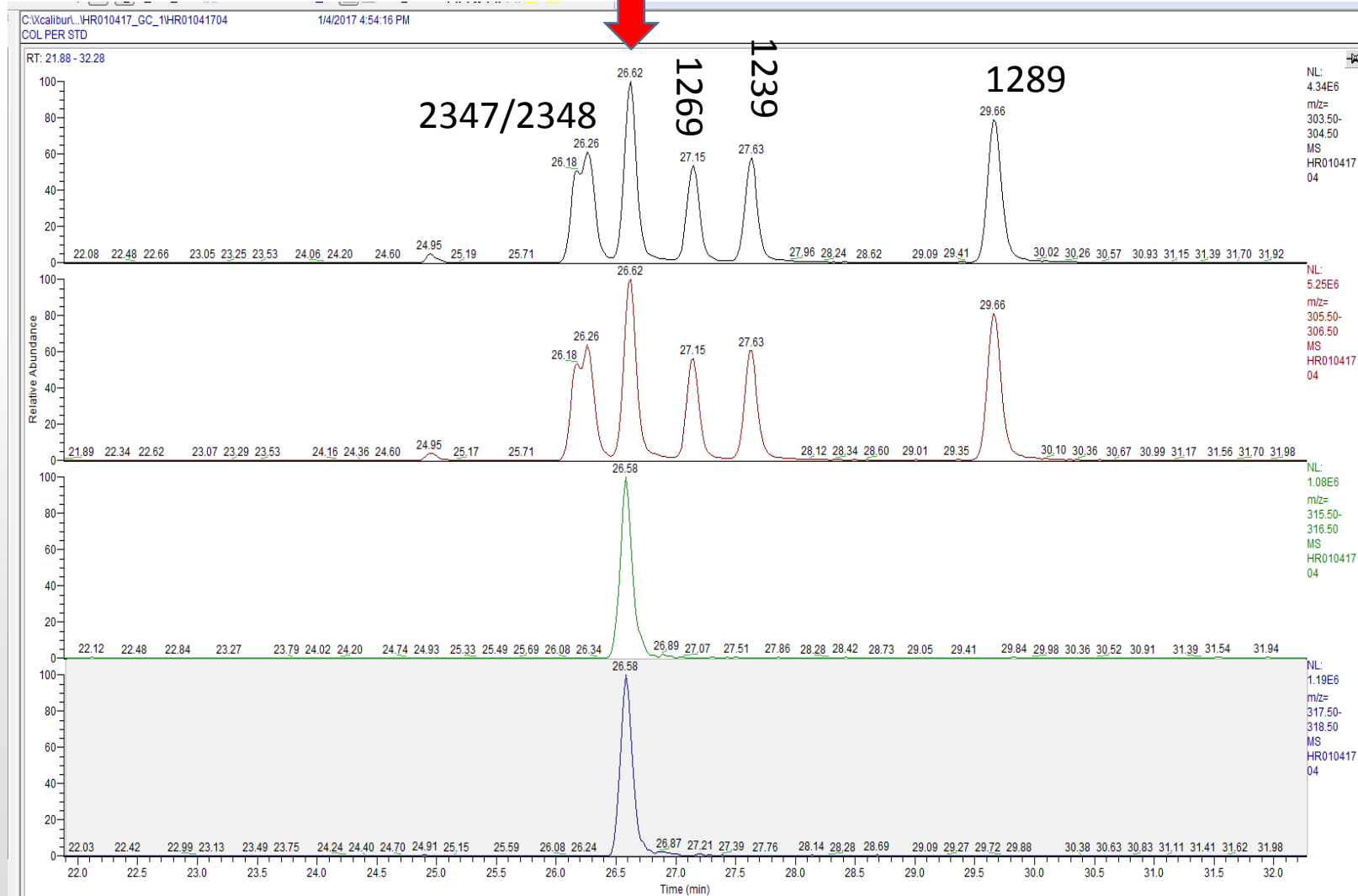
82% more samples!



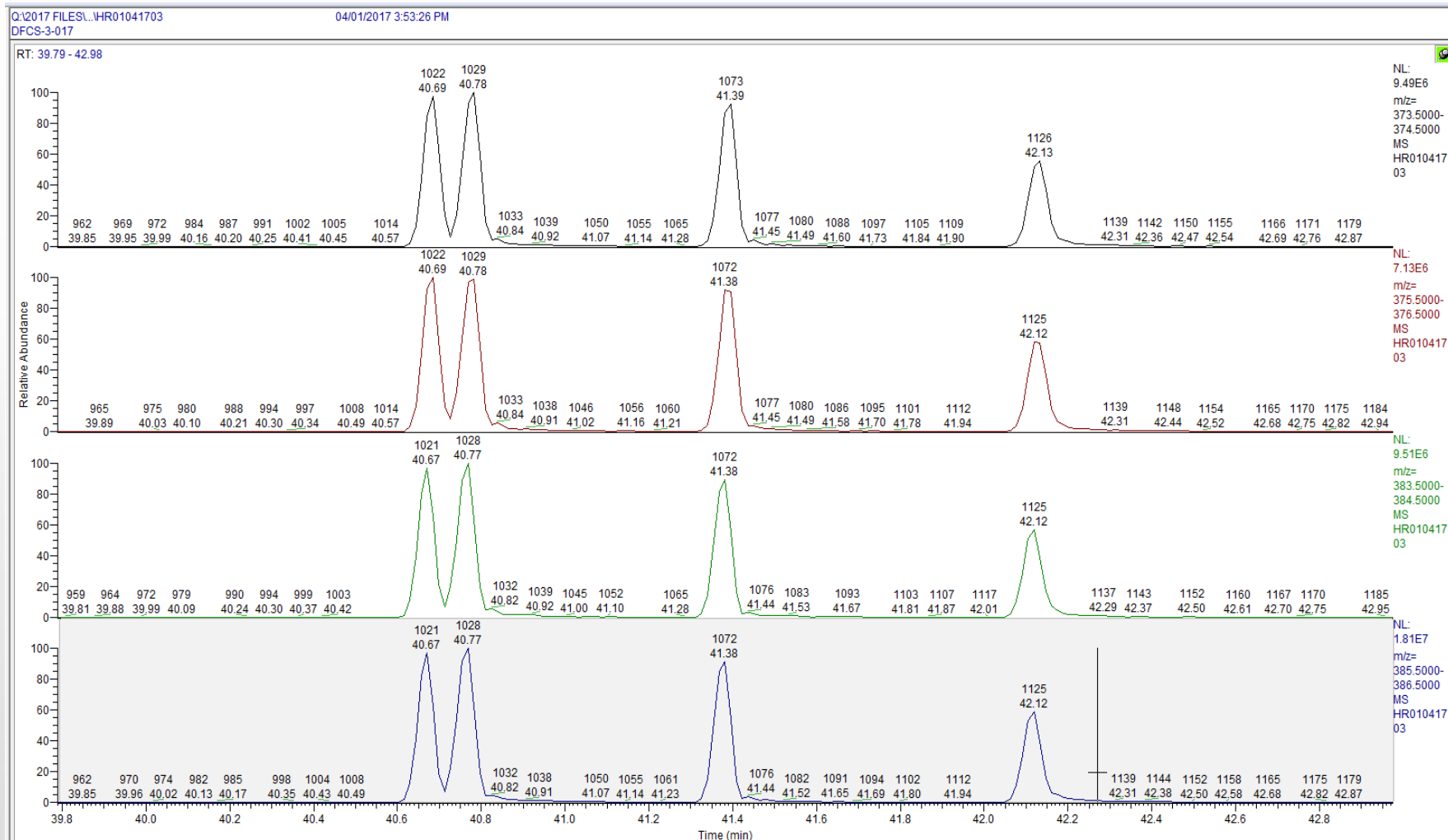
Column Resolution - TCDD



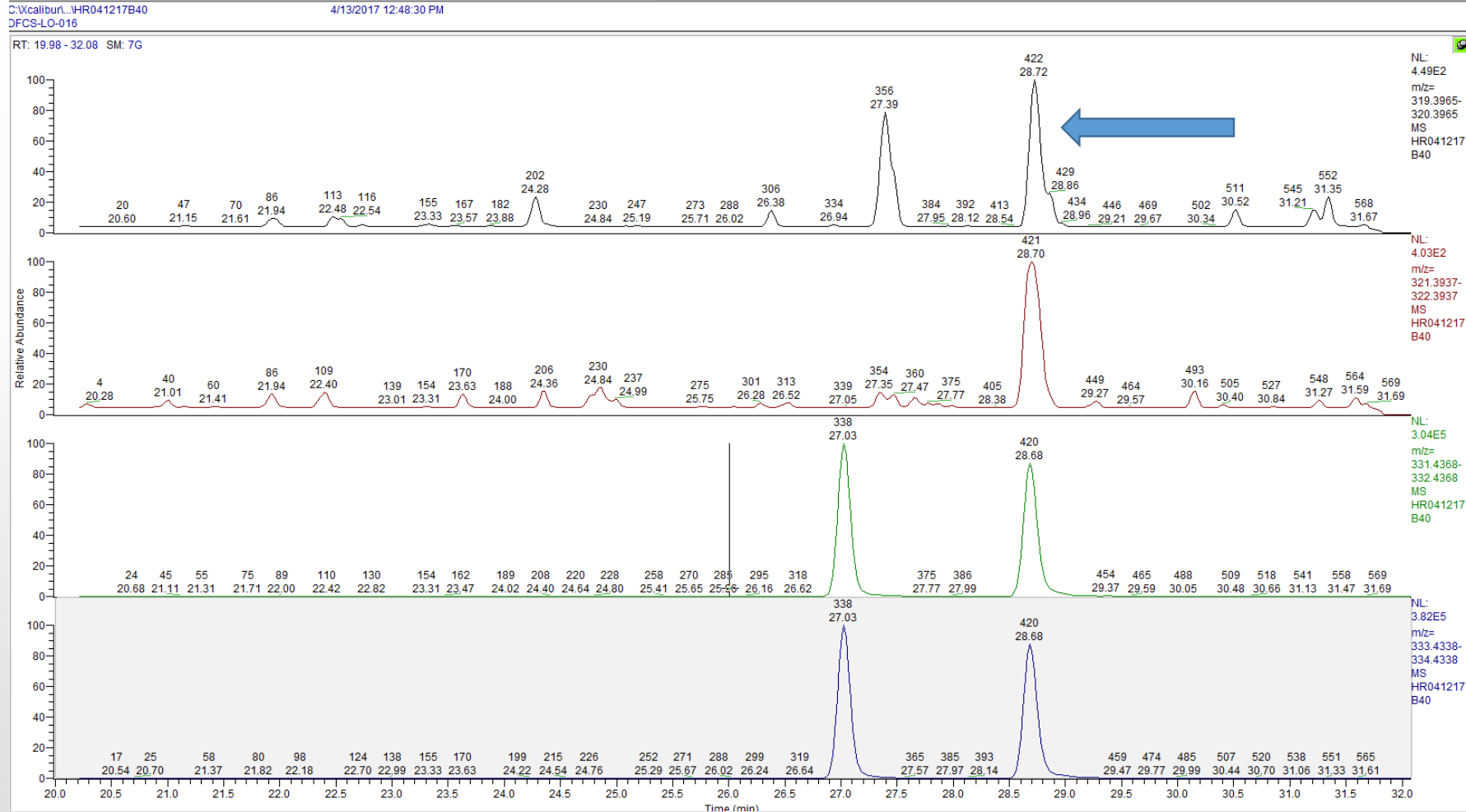
Resolution - TCDF



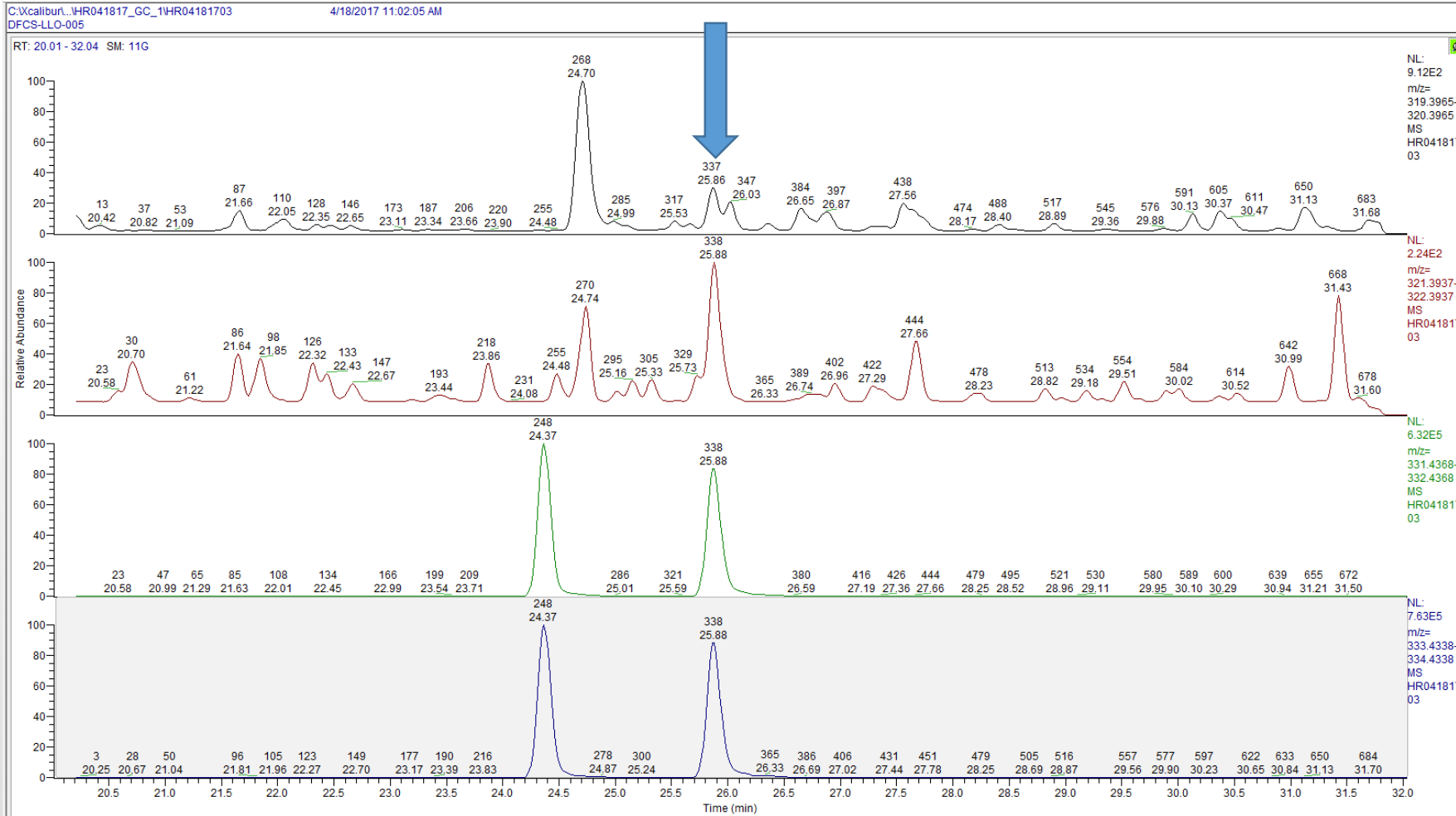
HxCDF resolution

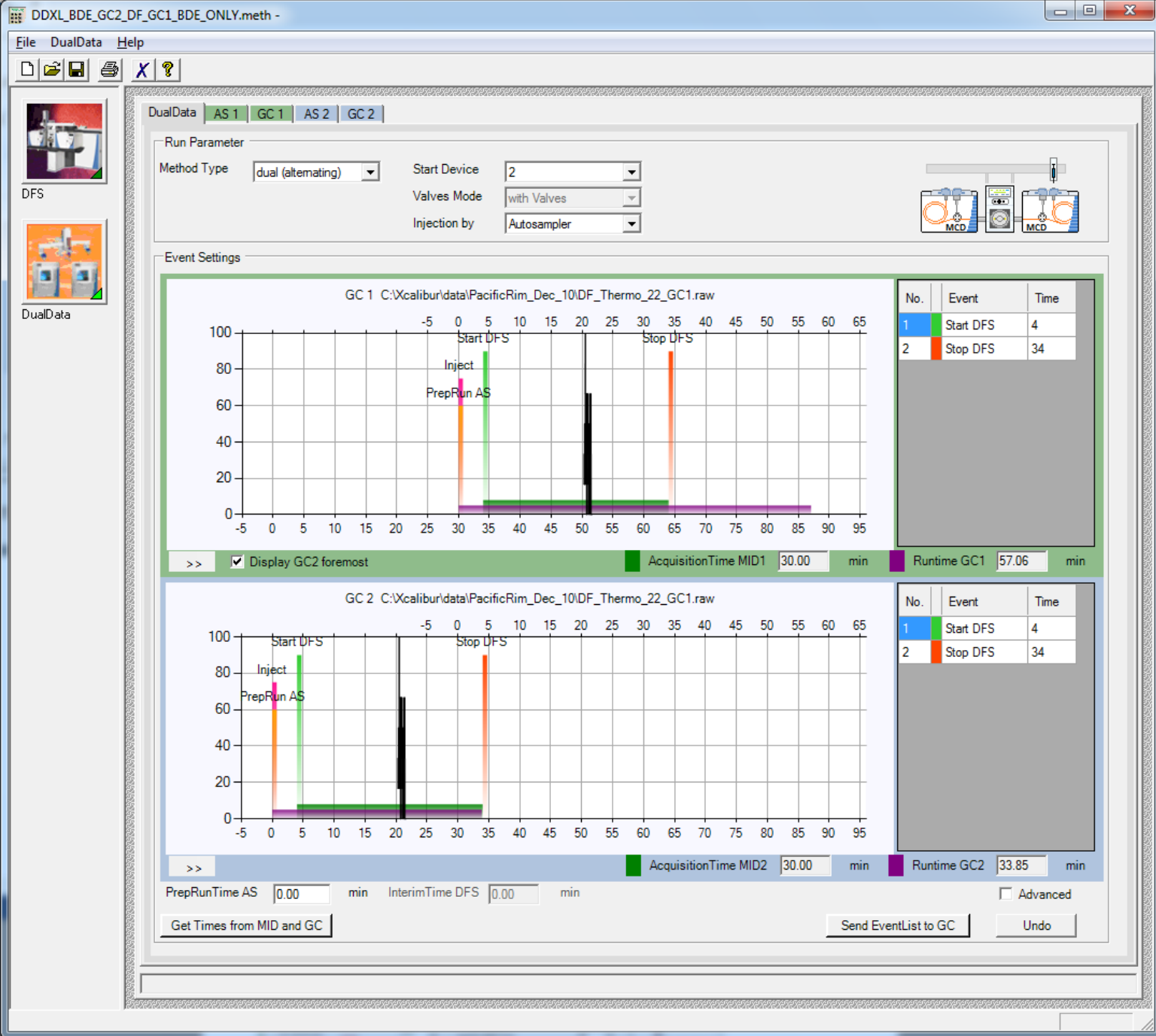


TCDD - CS-Lo 0.1 pg injected



TCDD – CS-LoLo! 20 fg injected





Dual BDE

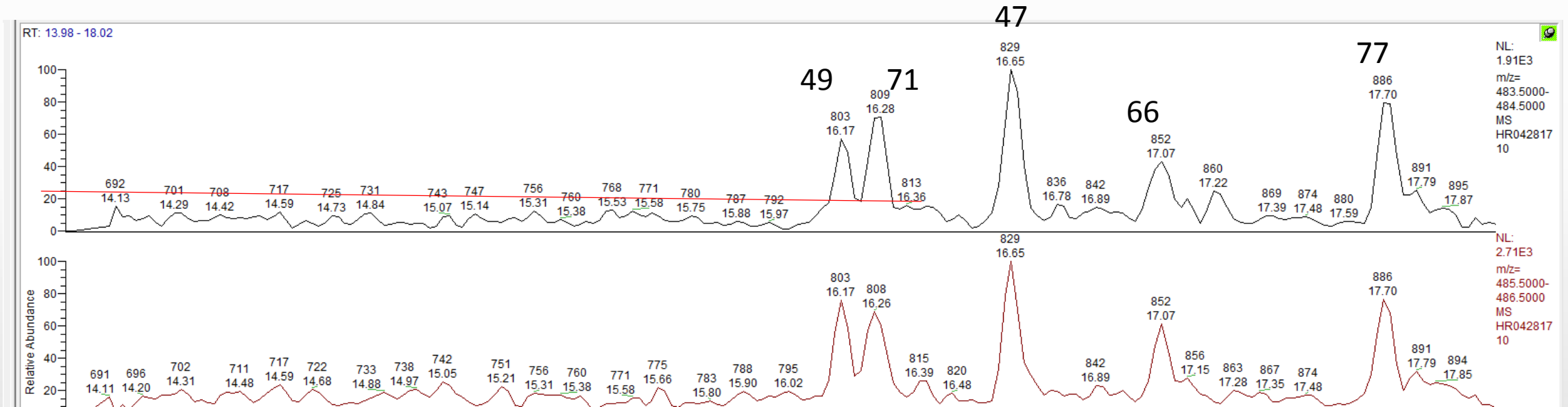
Runtime DFS – 41 minutes (35 inj/day)

Runtime DualData XL – 60 minutes (47 inj/day)

34% more runs!



TeBDE @ 0.5 pg injected

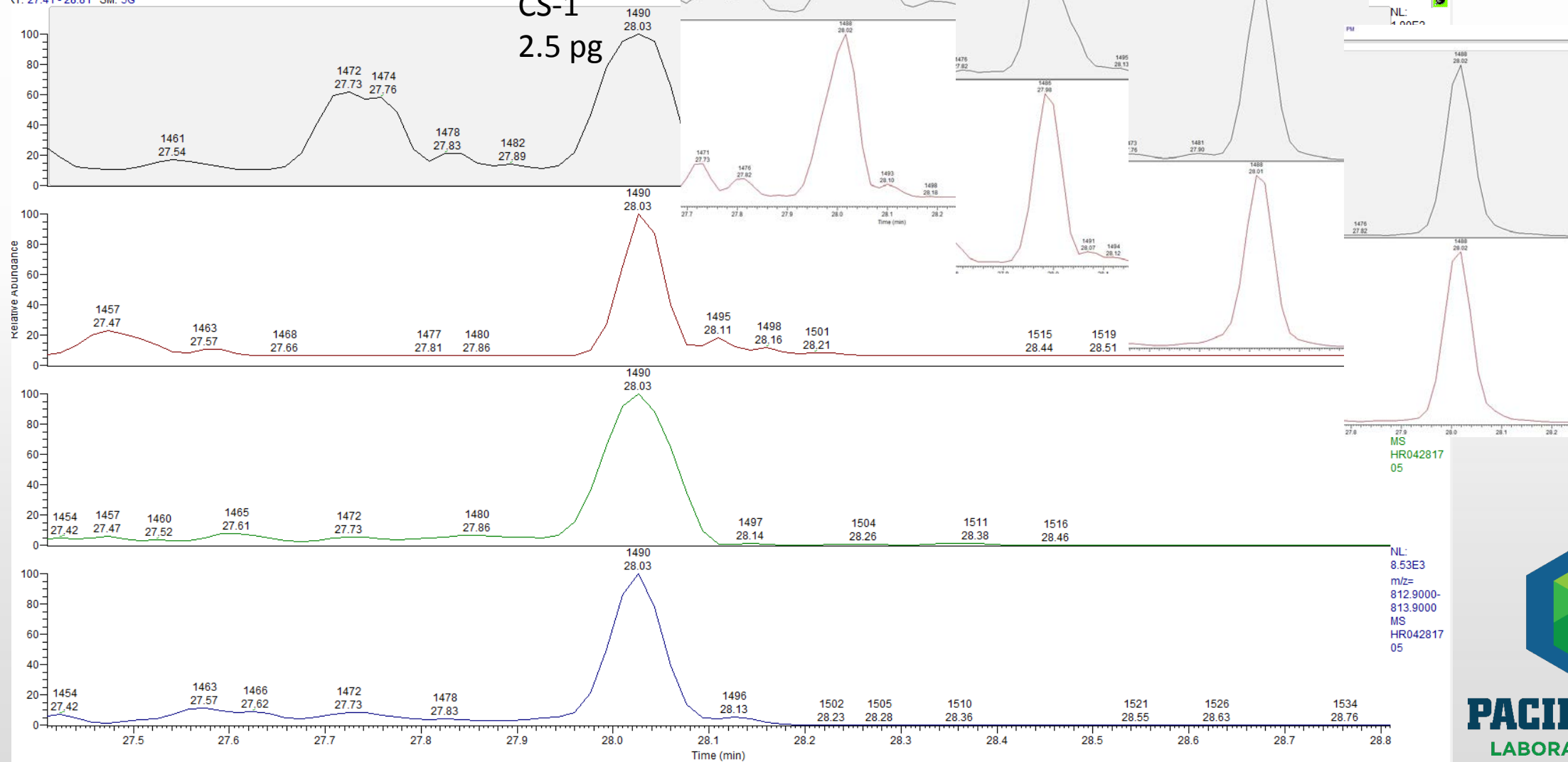


DecaDBE

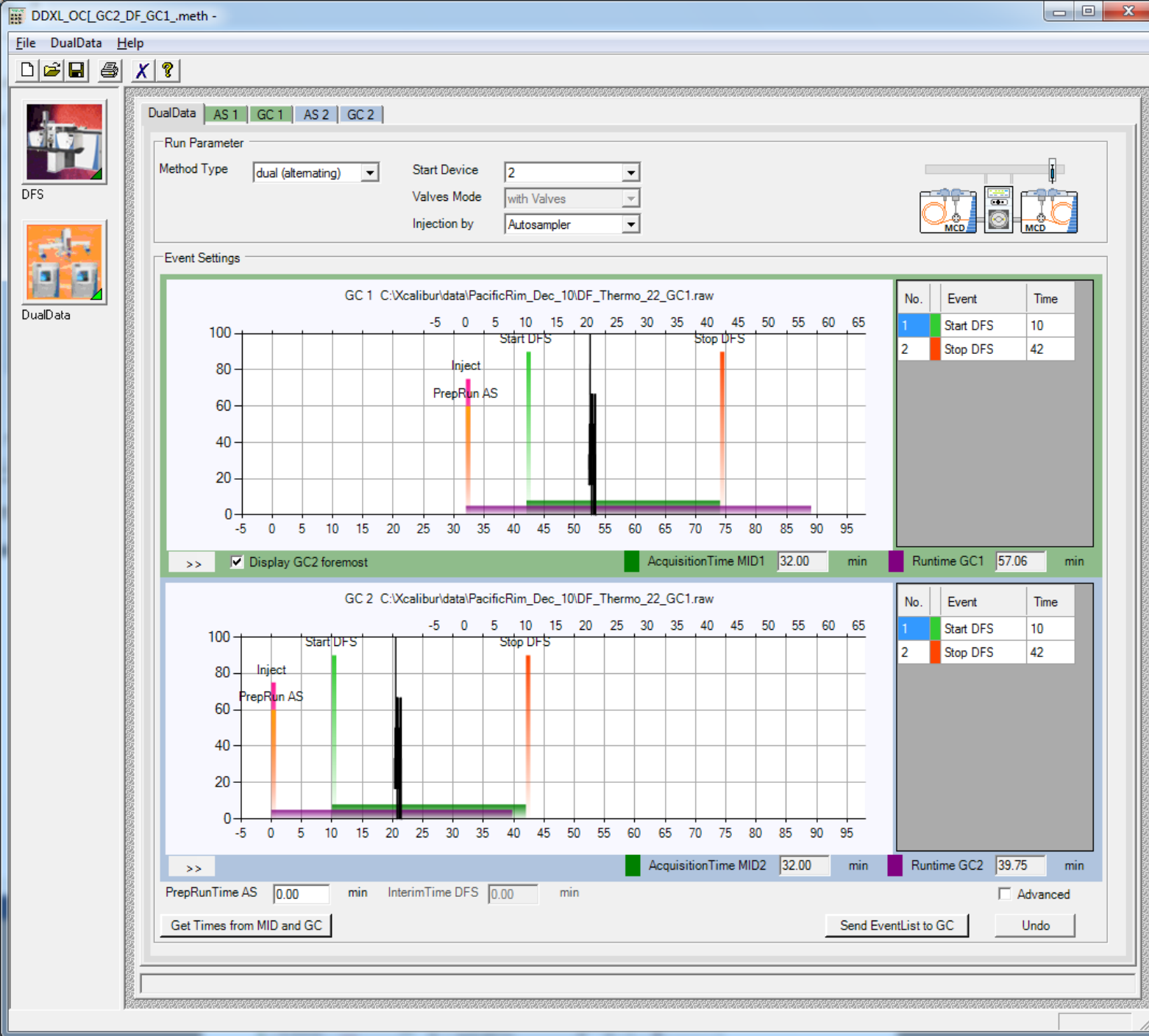
4/29/2017 3:25:02 PM

RT: 27.41 - 28.81 SM: 5G

CS-1
2.5 pg



PACIFIC RIM
LABORATORIES INC



Dual OCP

Runtime DFS – 51 minutes (28 inj/day)

Runtime DualData XL – 64 minutes (44 inj/day)

57% more analyses



PACIFIC RIM
LABORATORIES INC

Our workload is not just dioxins



- PCDD/F 21%
- PCB 23%
- PAH* 35%
- OCP 6%
- TBT* 7%
- PBDE 2%
- Other* 6%

• *mix of HRMS and MS/MS



PCDD/F & dIPCB

PCDD/F Runtime DFS – 62 minutes

The screenshot displays the Thermo Xcalibur Instrument Setup software interface. The main window is titled "DualData" and shows parameters for two GC channels (GC 1 and GC 2). The "Run Parameter" section includes Method Type (single), Start Device (2), Valves Mode (with Valves), and Injection by (Autosampler). The "Event Settings" section shows two chromatograms with their respective event logs.

GC 1 Event Log:

No.	Event	Time
1	Start DFS	13
2	Stop DFS	37

GC 2 Event Log:

No.	Event	Time
1	Start DFS	20
2	Stop DFS	53

Additional parameters shown include AcquisitionTime MID1 (24.00 min), Runtime GC1 (37.93 min), AcquisitionTime MID2 (33.00 min), and Runtime GC2 (57.06 min). The interface also includes buttons for "Get Times from MID and GC", "Send EventList to GC", and "Undo".

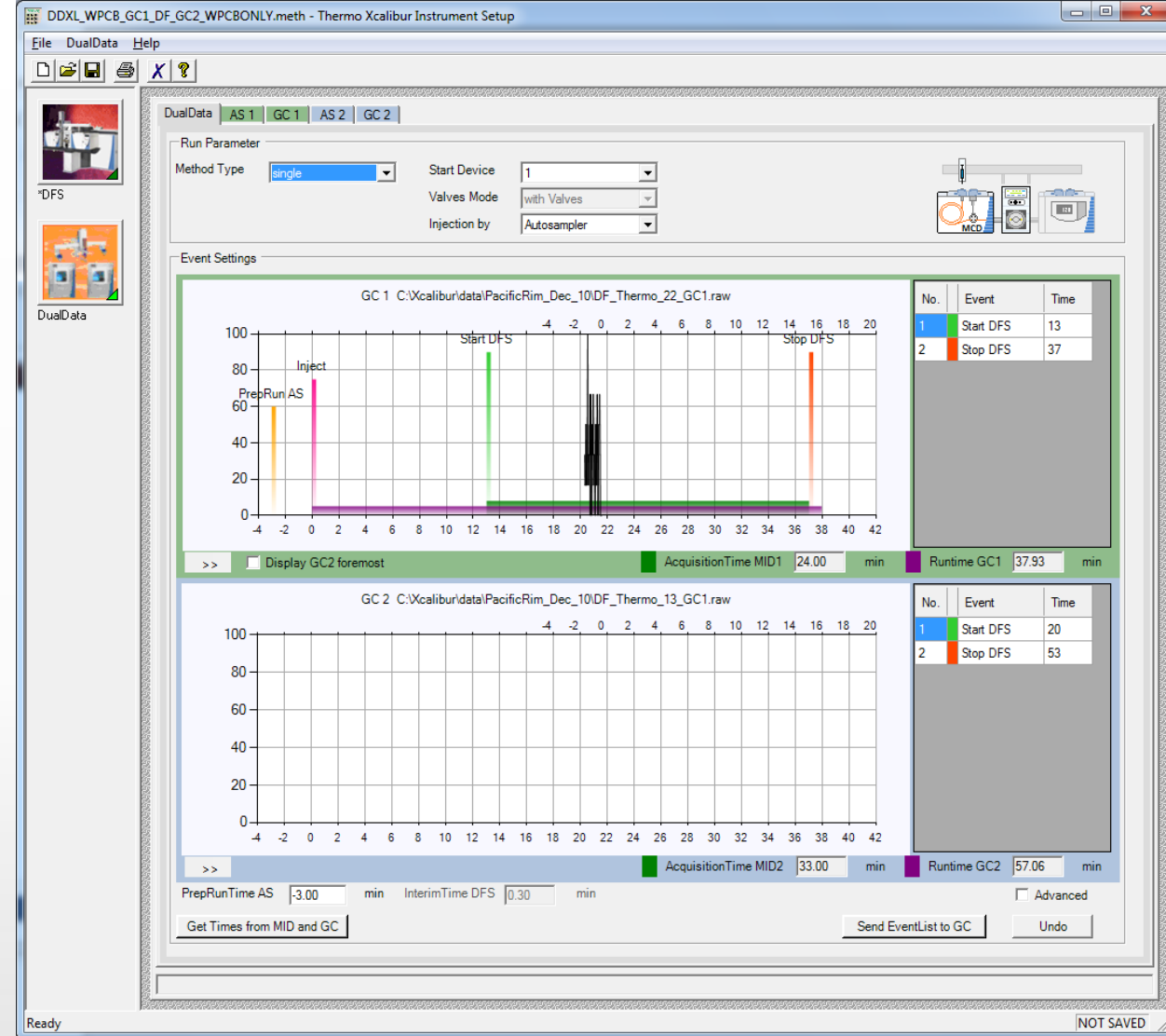


PACIFIC RIM
LABORATORIES INC

PCDD/F & dIPCB

PCDD/F Runtime DFS – 62 minutes

PCB Runtime DFS – 48 minutes



PACIFIC RIM
LABORATORIES INC

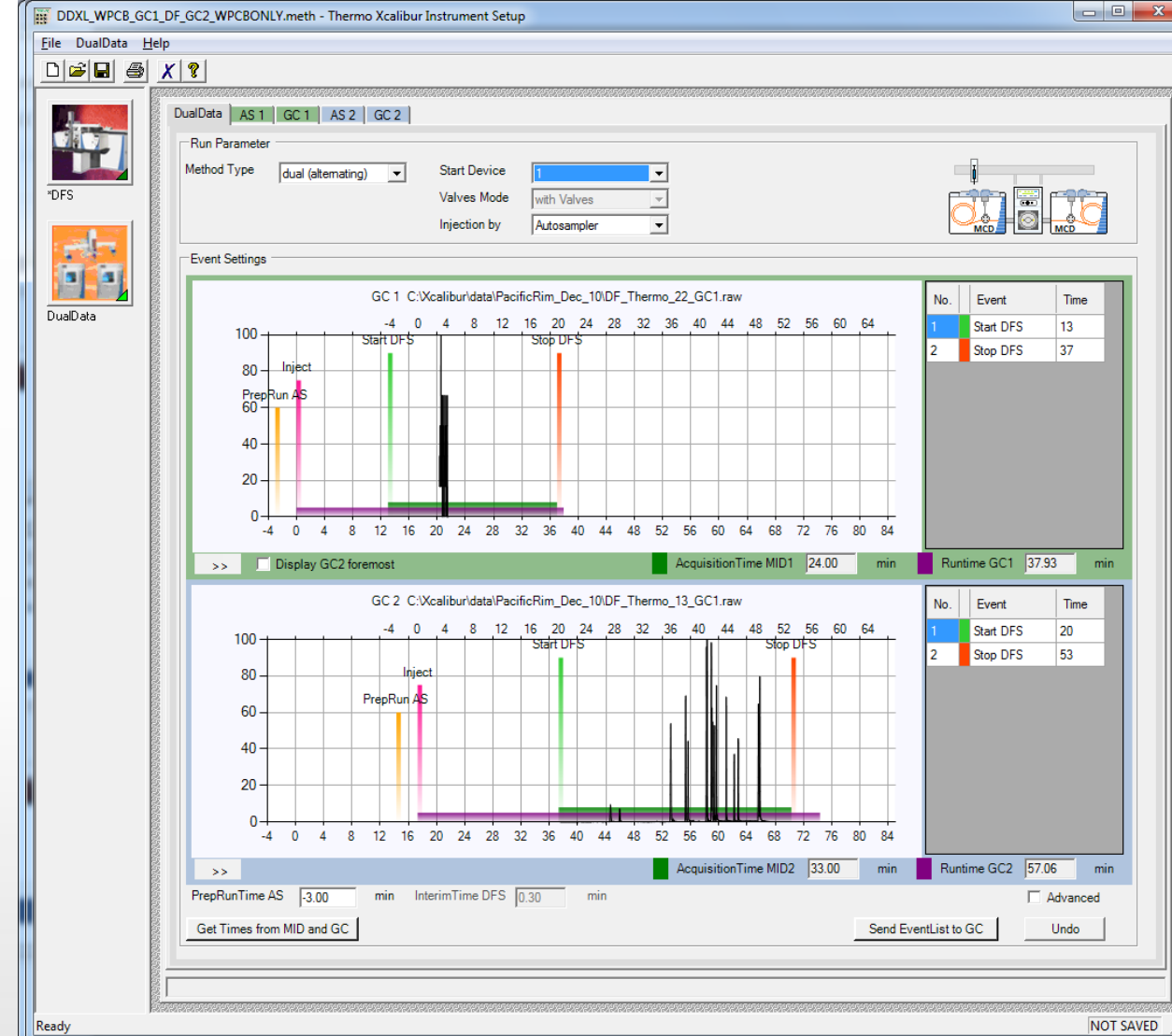
PCDD/F & dIPCB

PCDD/F Runtime DFS – 62 minutes

PCB Runtime DFS – 48 minutes

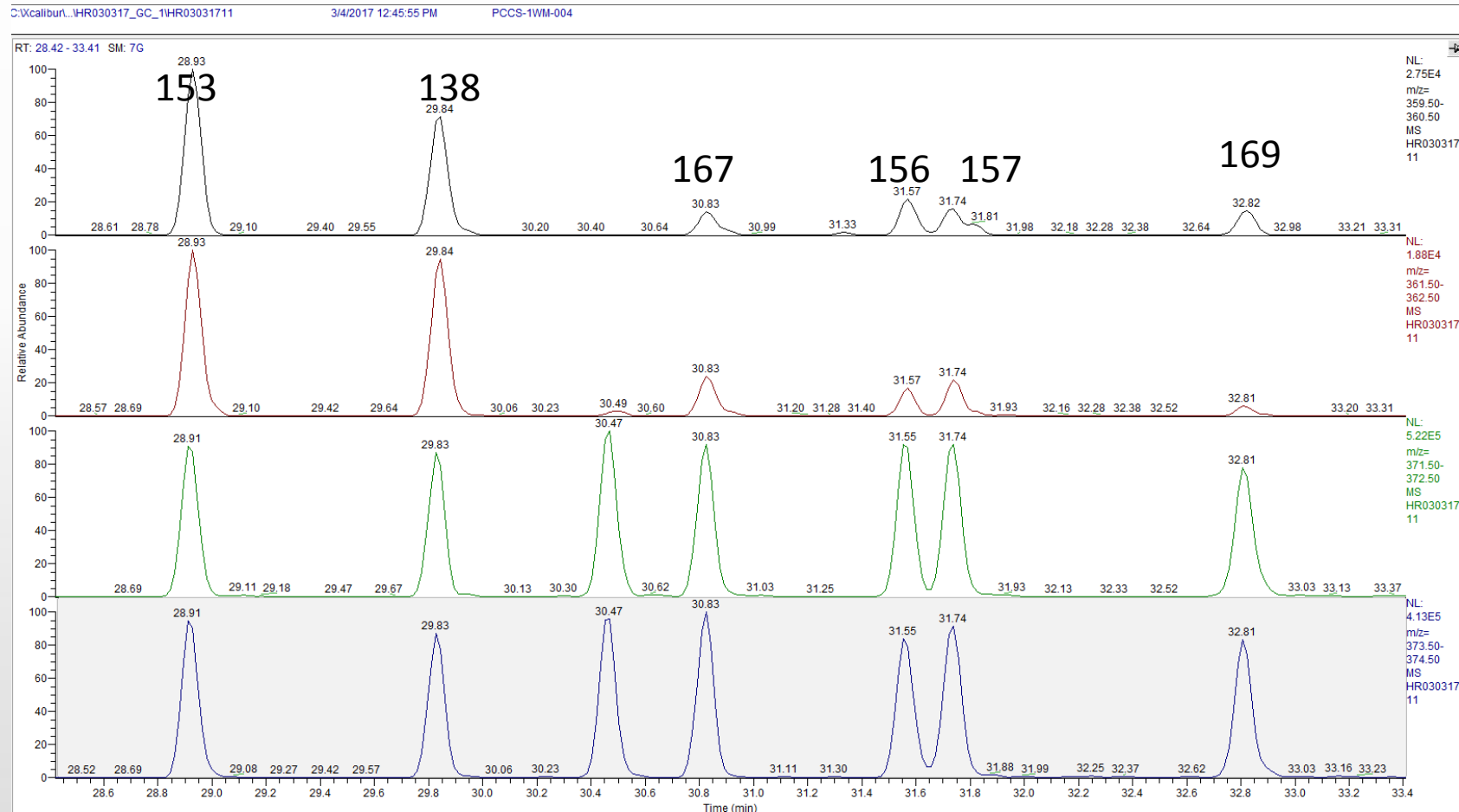
Runtime DualData XL – 57 minutes

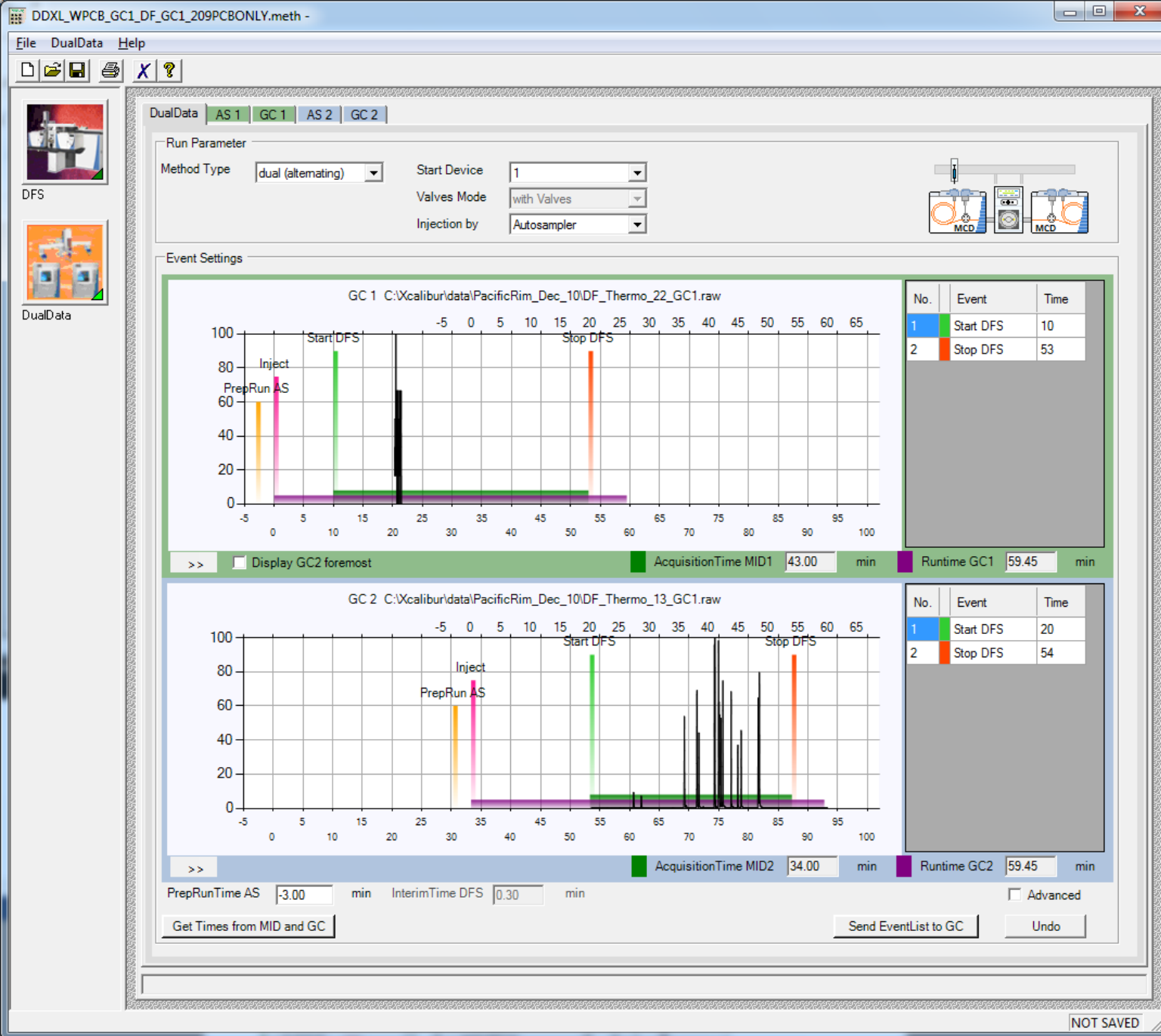
Therefore, you can run dioxins and PCBs together in less time than it takes to run one dioxin sample!!!



PACIFIC RIM
LABORATORIES INC

HxCB @ 0.1/0.5 pg injected





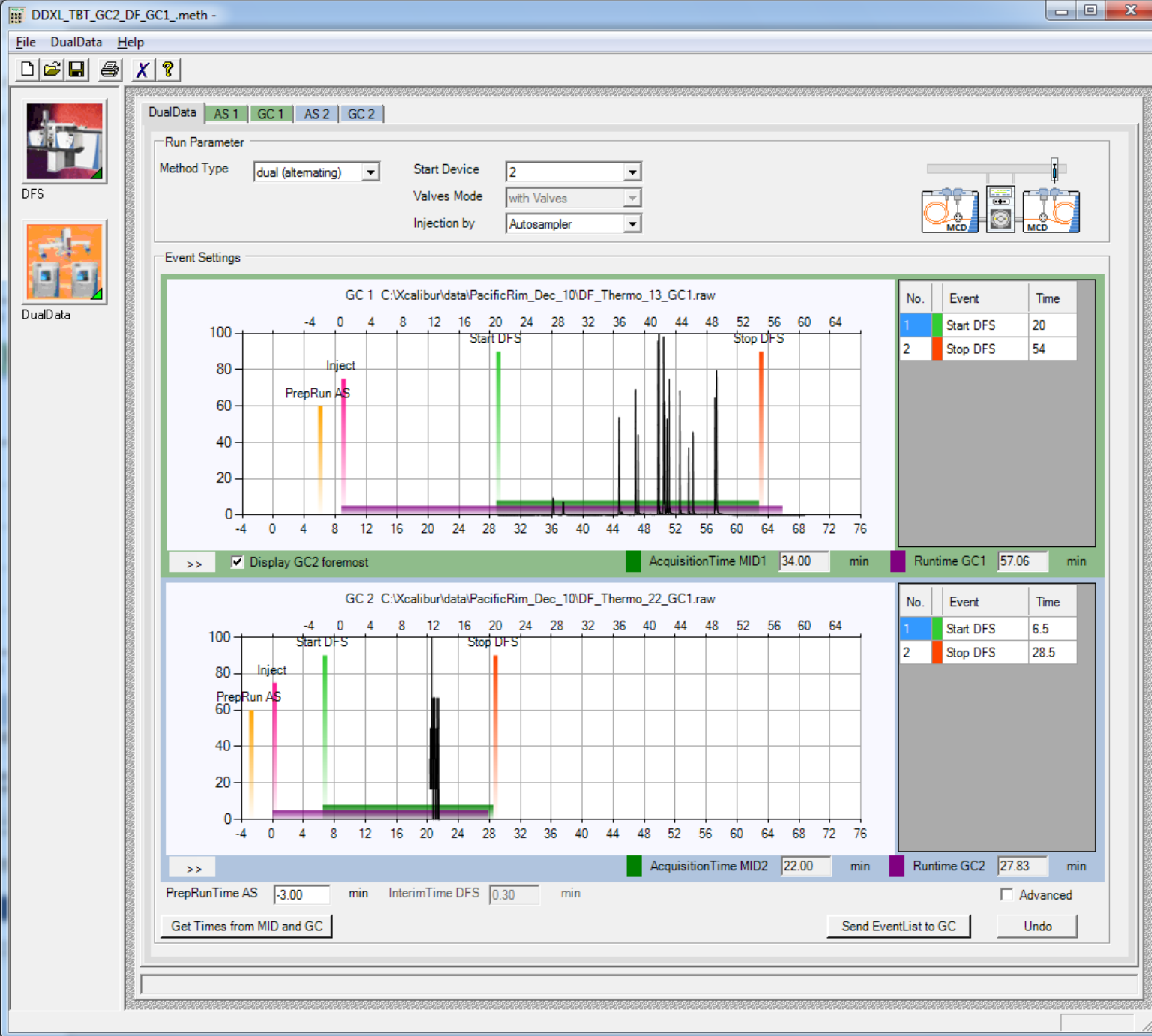
PCDD/F and 209 congener PCB

PCDD/F Runtime DFS – 62 minutes

PCB Runtime DFS – 69 minutes
(EPA1668C: PCB209 cannot elute before 55 minutes)

Runtime DualData XL – 77 minutes





PCDD/F & TBT

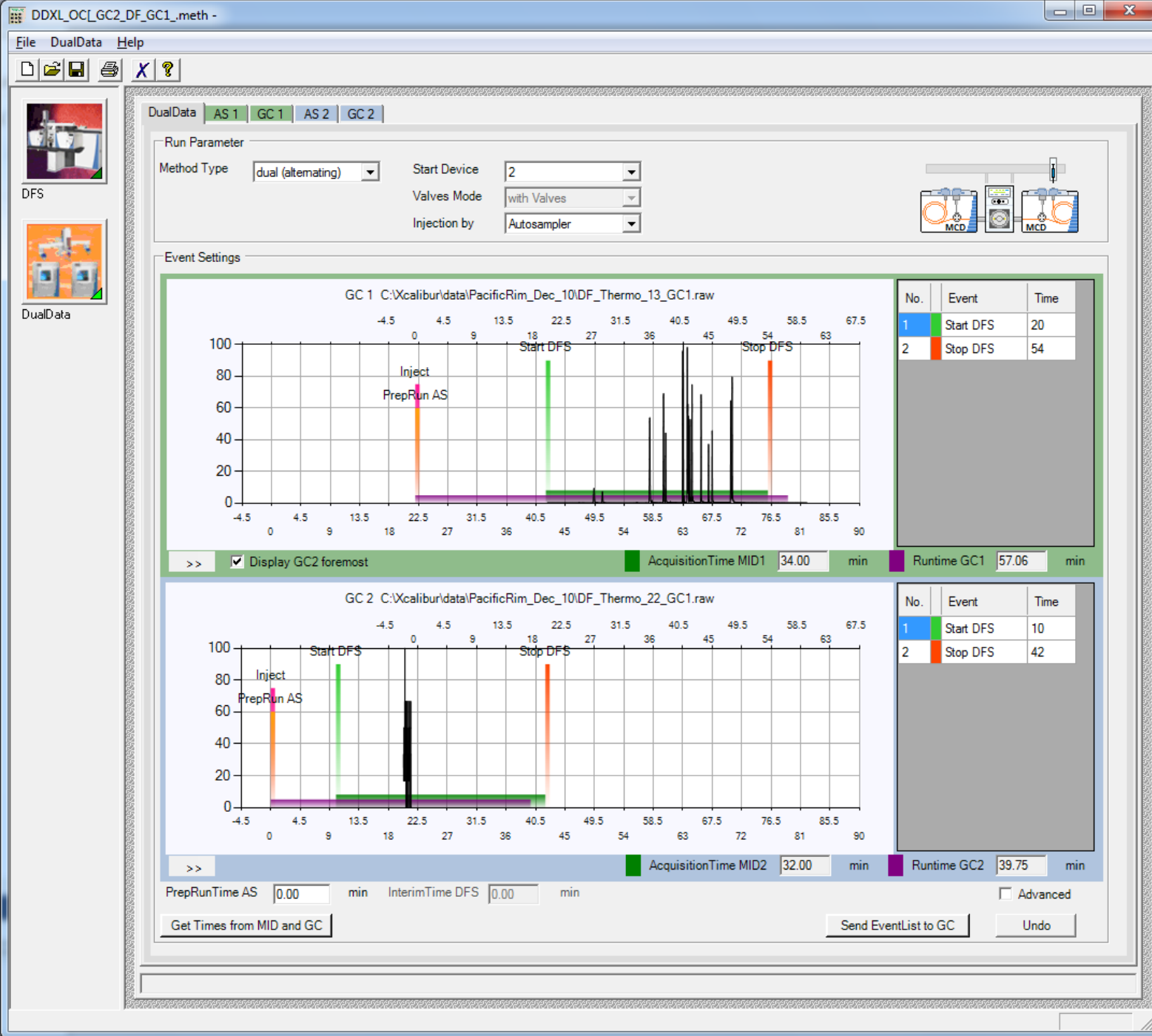
PCDD/F Runtime DFS – 62 minutes

TBT Runtime DFS – 30 minutes

Runtime DualData XL – **56 minutes***

* This takes less time than running dioxins by themselves!!





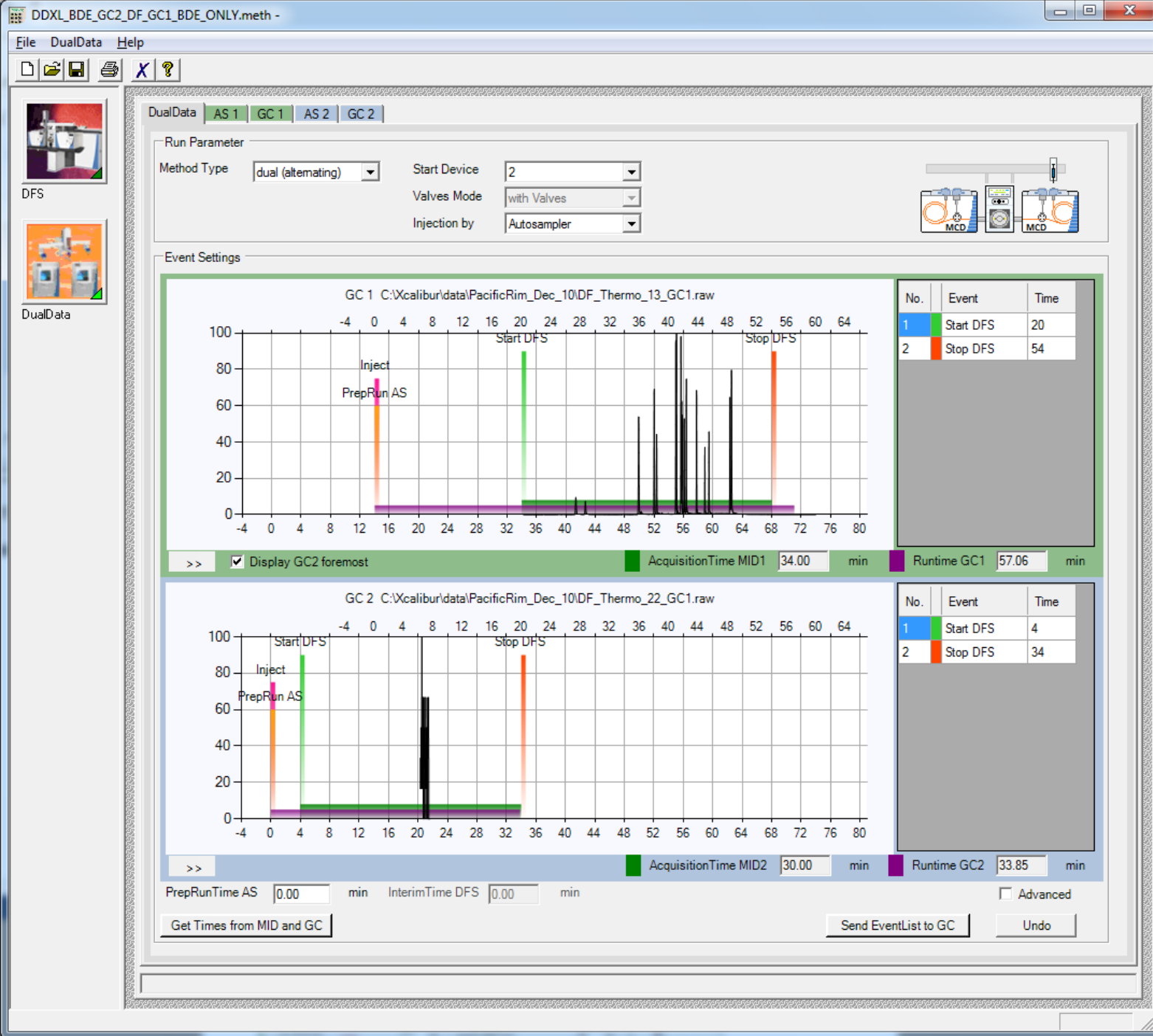
PCDD/F & OCP

PCDD/F Runtime DFS – 62 minutes

OCP Runtime DFS – 51 minutes

Runtime DualData XL – 66 minutes





PCDD/F and PBDE

PCDD/F Runtime DFS – 62 minutes

PBDE Runtime DFS – 41 minutes

Runtime DualData XL – 64 minutes

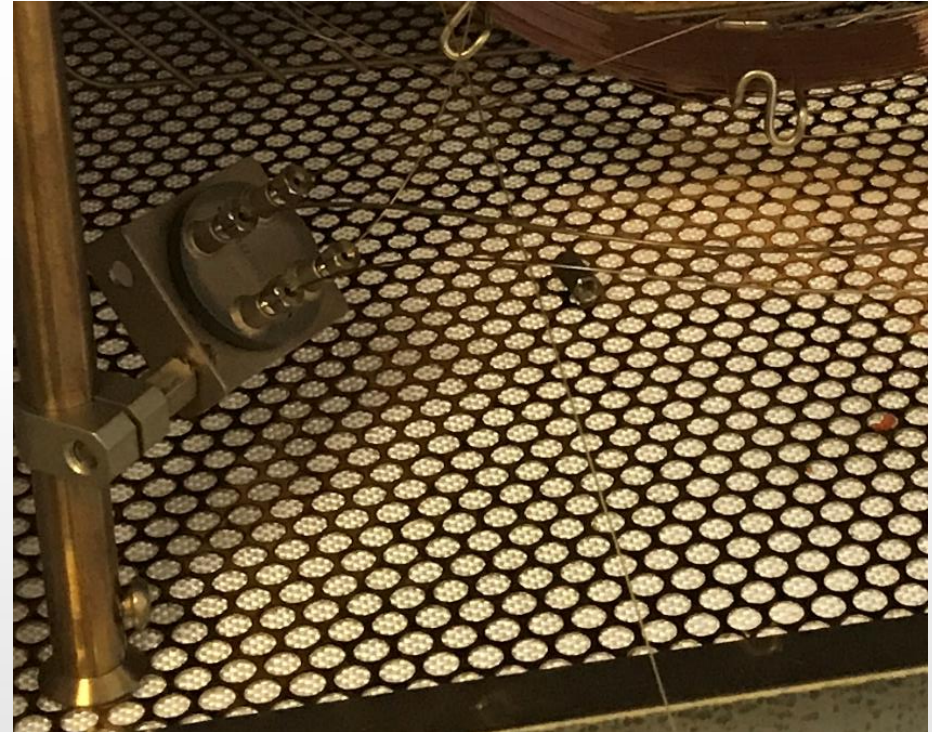
Note – you must run PBDE at 10,000 resolution

In our lab we use different tuning compound for PBDE v dioxin, so would never run together. This is just an example of what could be done.



Conclusions

1. DualData XL saves time, even when running in single GC mode
2. Not limited to running the same column/program in each GC
3. Source changes less frequent as “burn off” being vented to air
4. Wafers are a consumable, but are cleanable too!
5. Source does not need to be vented when changing columns



DI **XIN 2017**

Vancouver, Canada

August 20 -25, 2017

www.dioxin2017.org



PACIFIC RIM
LABORATORIES INC

Thank you from Pacific Rim Labs.



PACIFIC RIM
LABORATORIES INC