100th Anniversary of Regaining Independence by Poland

38th International Symposium on Halogenated Persistent Organic Pollutants

DioXin 2018

& 10th International PCB Workshop

26 – 31 August 2018, Kraków, Poland

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


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# Overview

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

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# Our first HRMS - VG70 arrives!

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# Beginnings

**Dioxin 2005 - Toronto**


**Thermo POPs Symposium– Venice 2007**

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# 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

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# 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)

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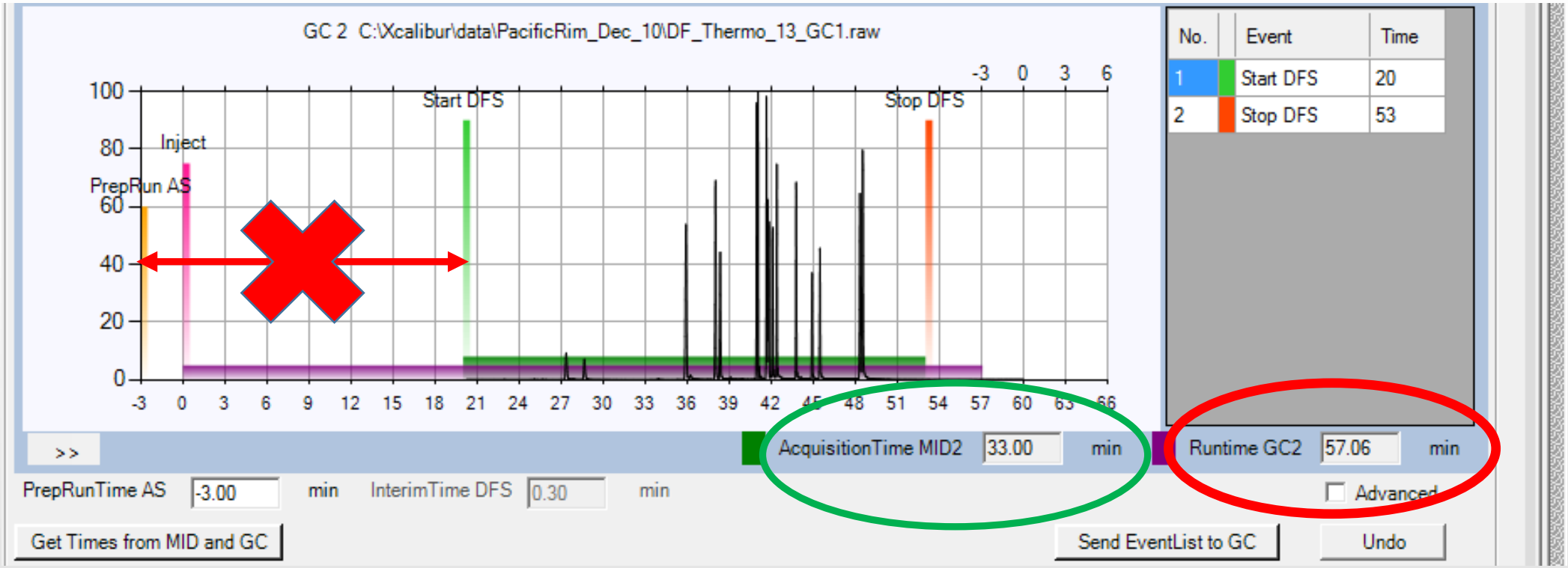
# What is Dual Data? PCDD/F analysis
# EPA 1613b – TCDD must elute >25 minutes

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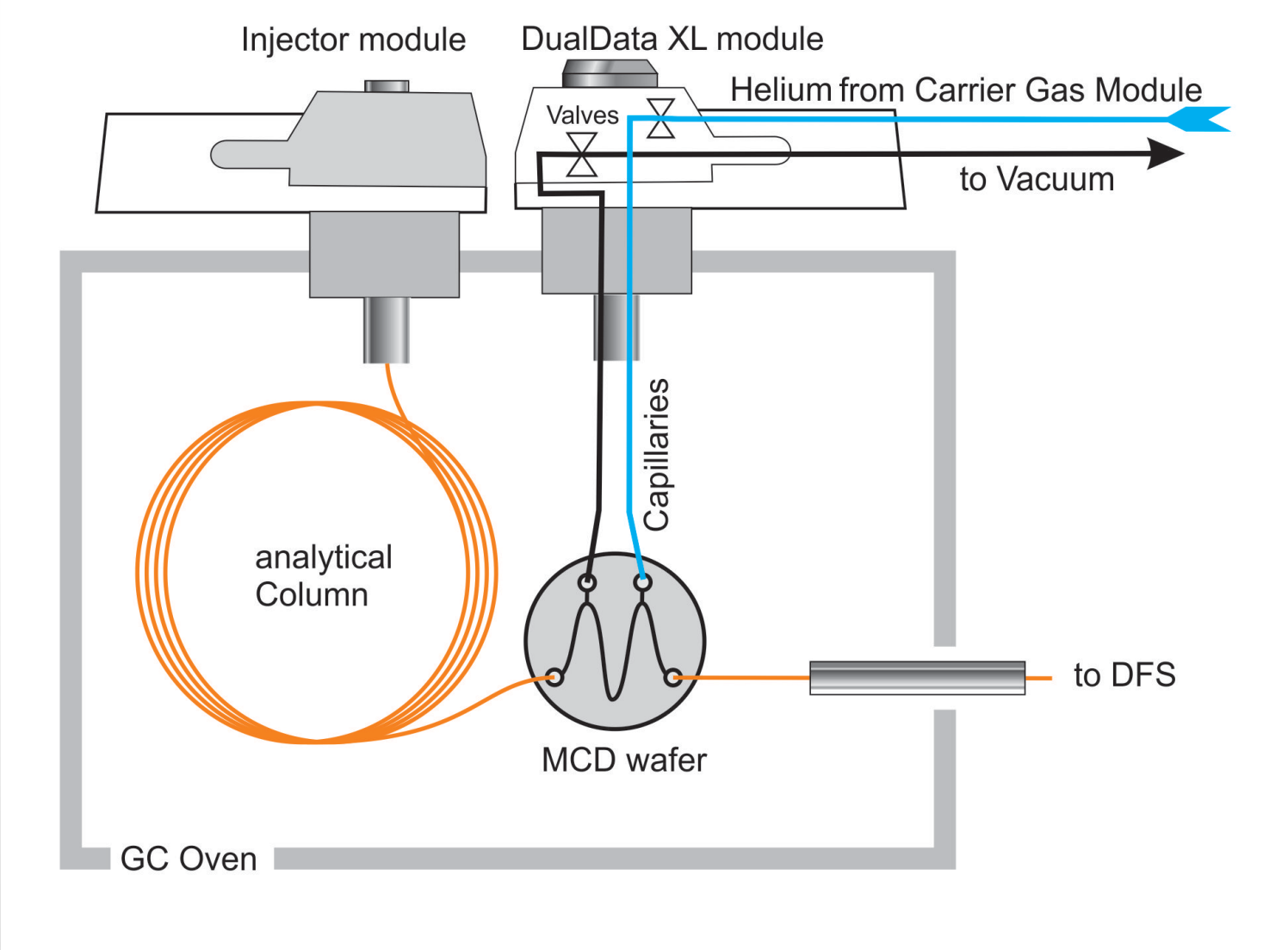


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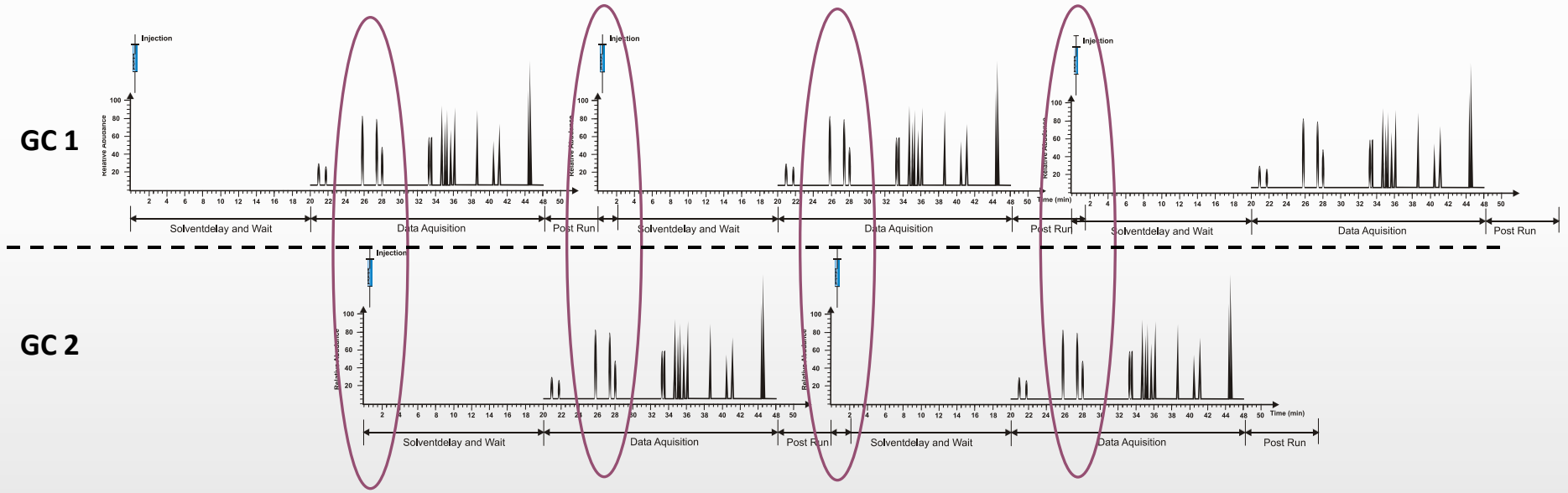
# DFS DualData XL: Staggered Injection

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

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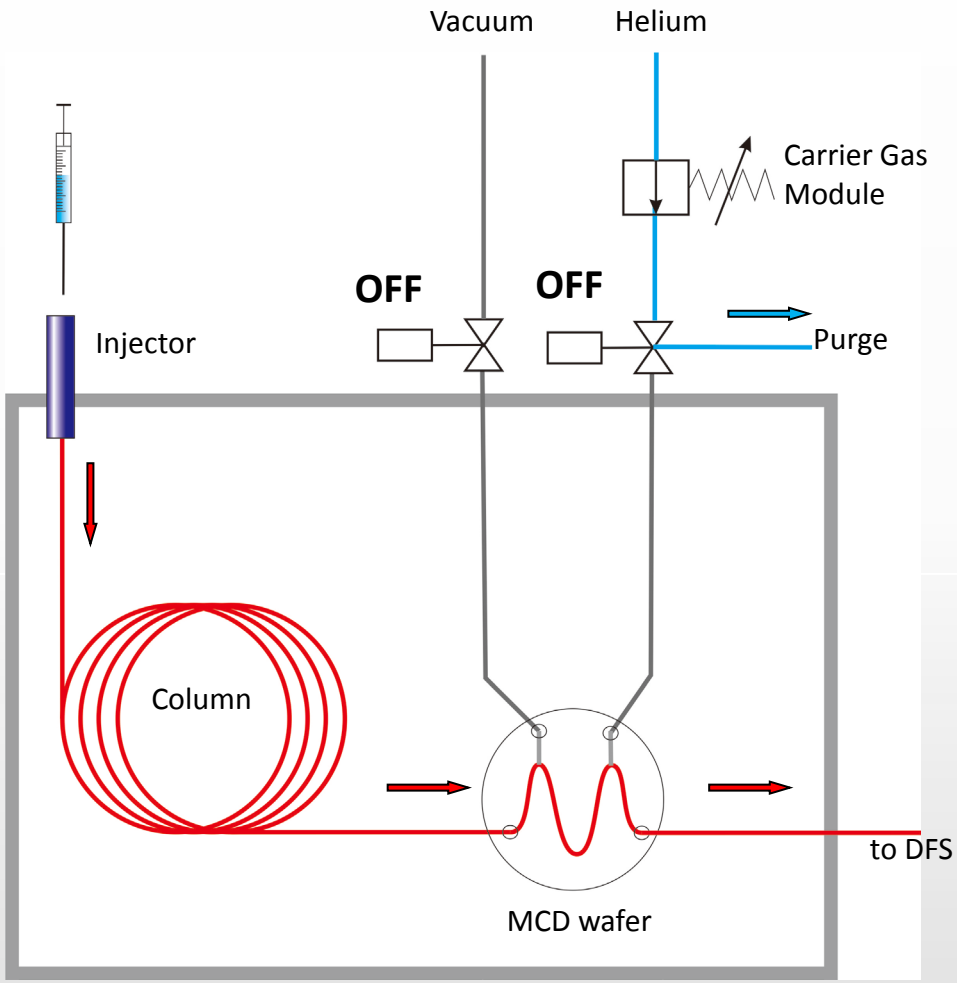
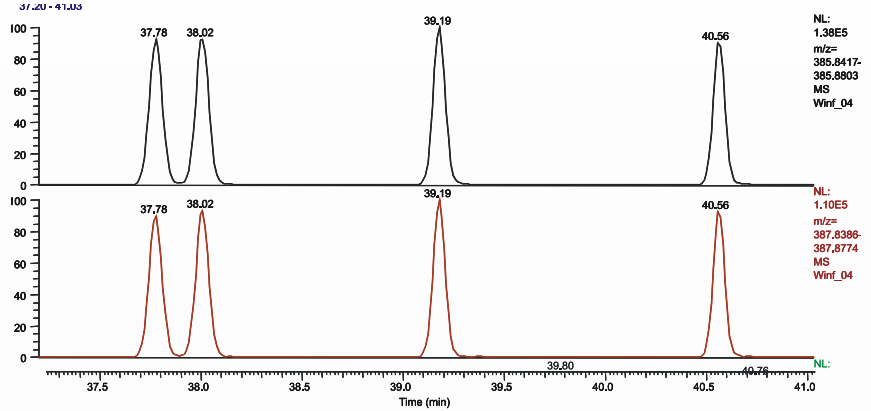
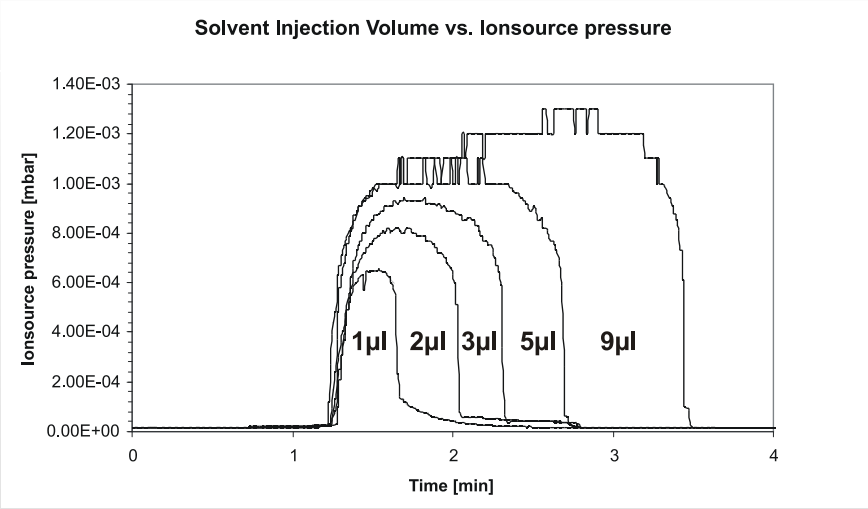
# Flow switching 1: Column-flow is directed into the MS




Example Standard inj.




Source pressure eq. Solvent inj.

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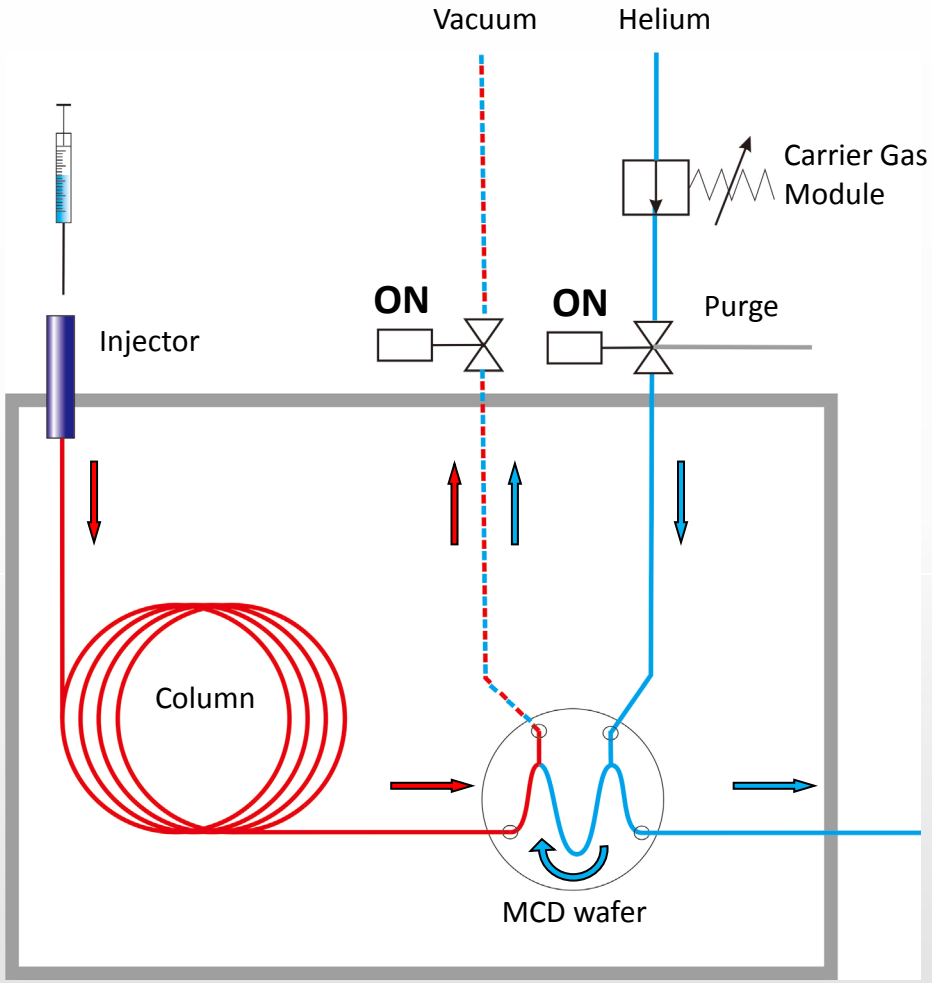
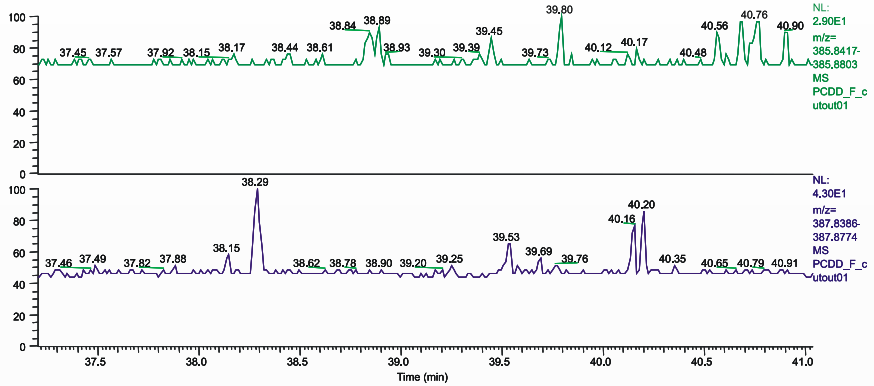
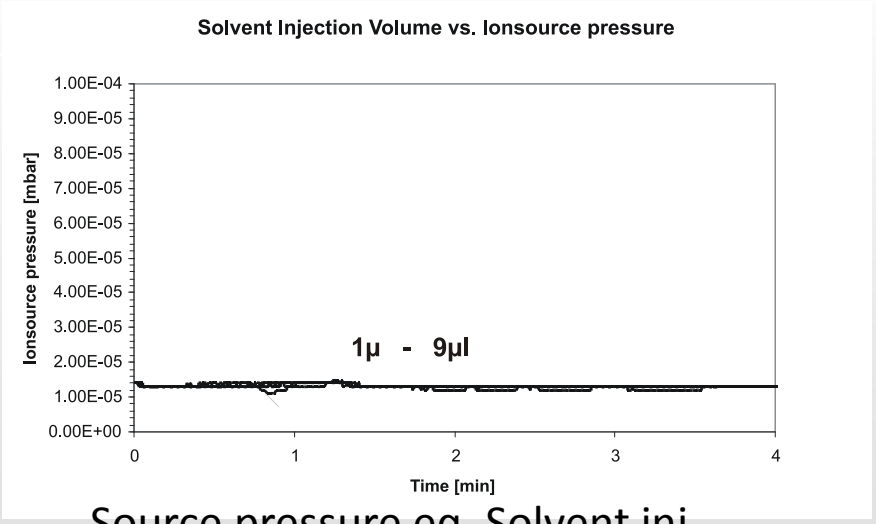
# Flow switching 2: Flow directed into service vacuum (waste)




Example Standard inj.




Source pressure eq. Solvent inj.

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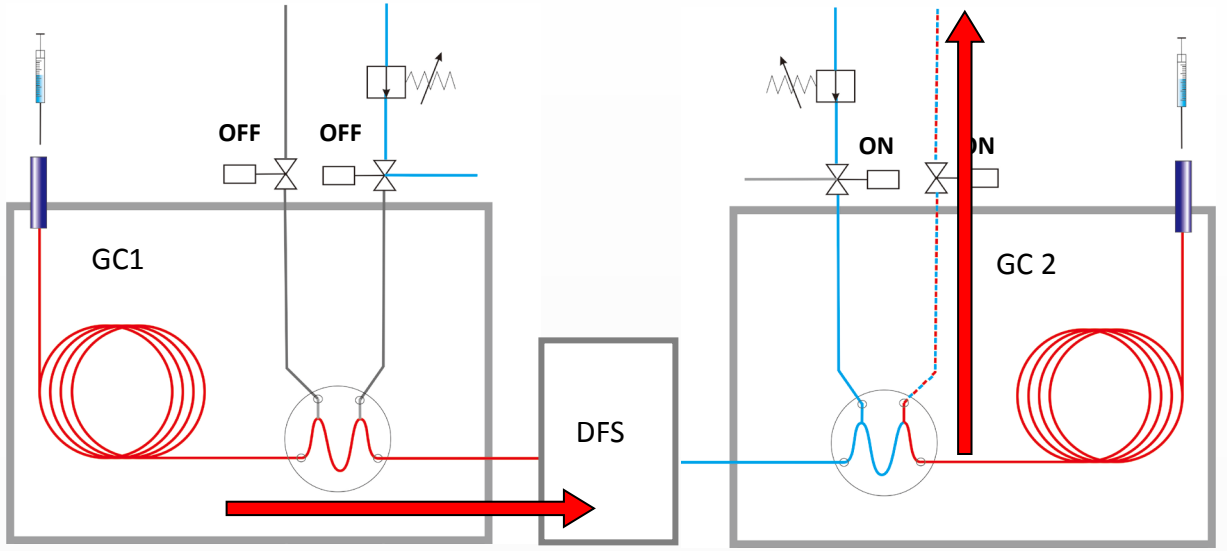
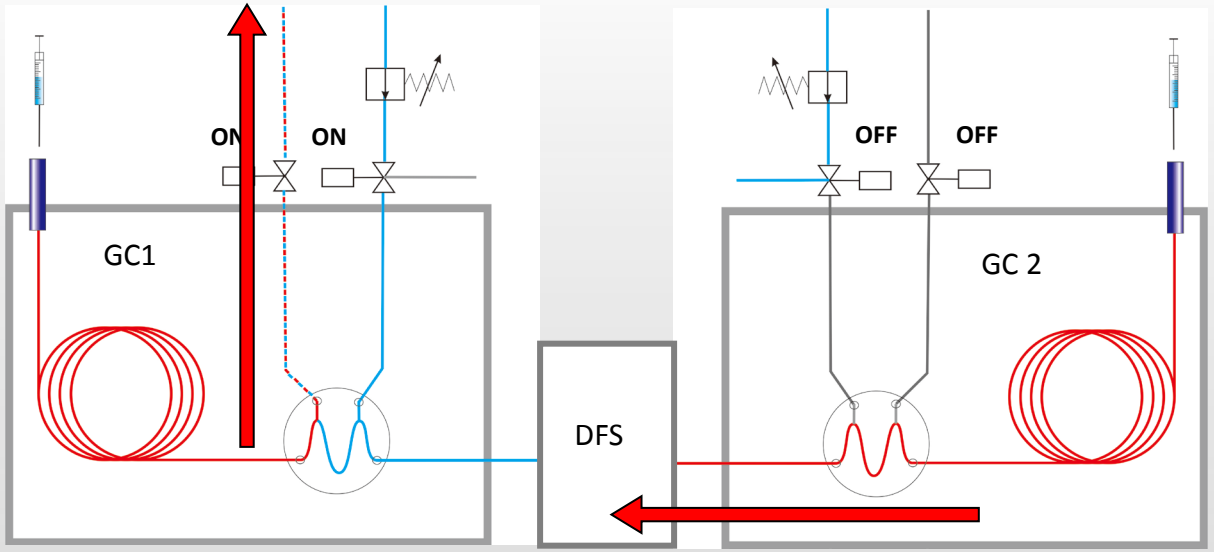
# Alternating Flow switching with both GCs

- **A:** Acquisition GC1
  - GC1 into MS
  - GC2 into waste




- **B:** Acquisition GC2
  - GC2 into MS
  - GC1 into waste

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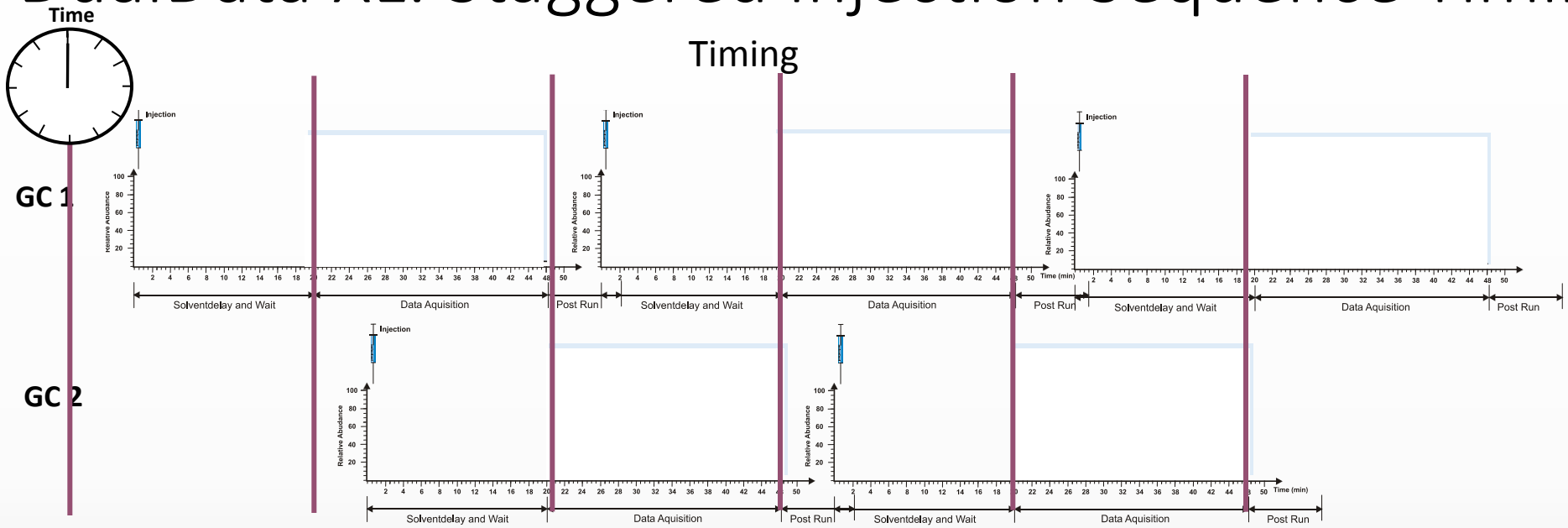
# DFS DualData XL: Staggered Injection Sequence Timing





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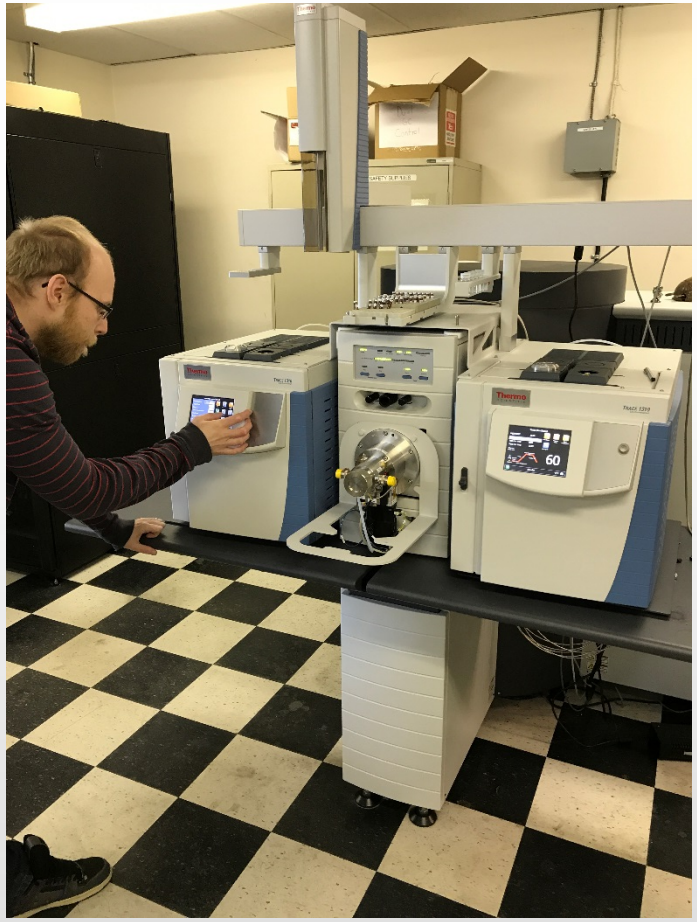
# Why DualData XL?



- 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

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# Requirements

- DFS with dual 1310 GCs
- Older DFS can be converted, but cannot use Trace GCs.
- Will add a 4-way valve to control gases
- A gas module is installed next to your injector.
- New software

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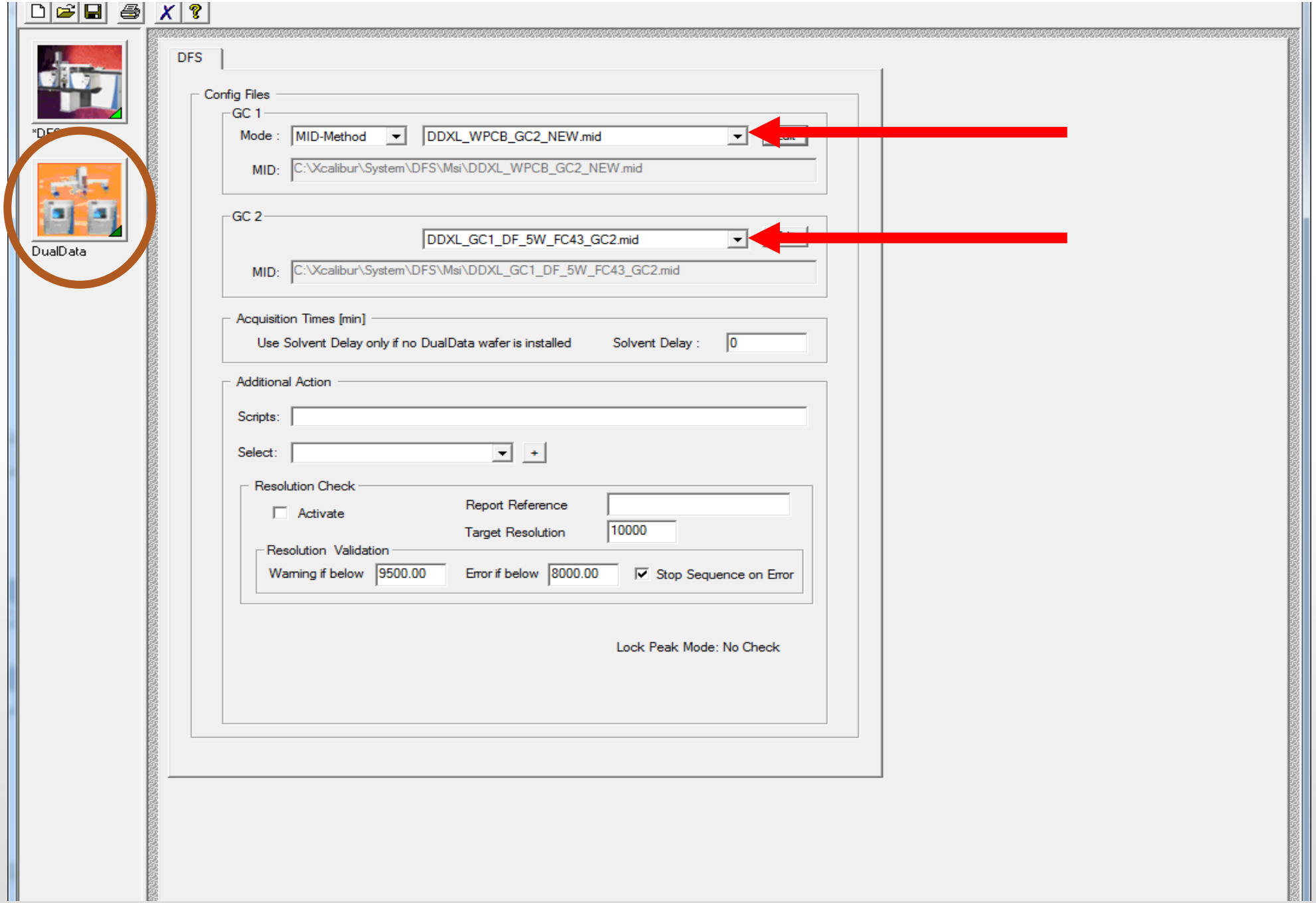


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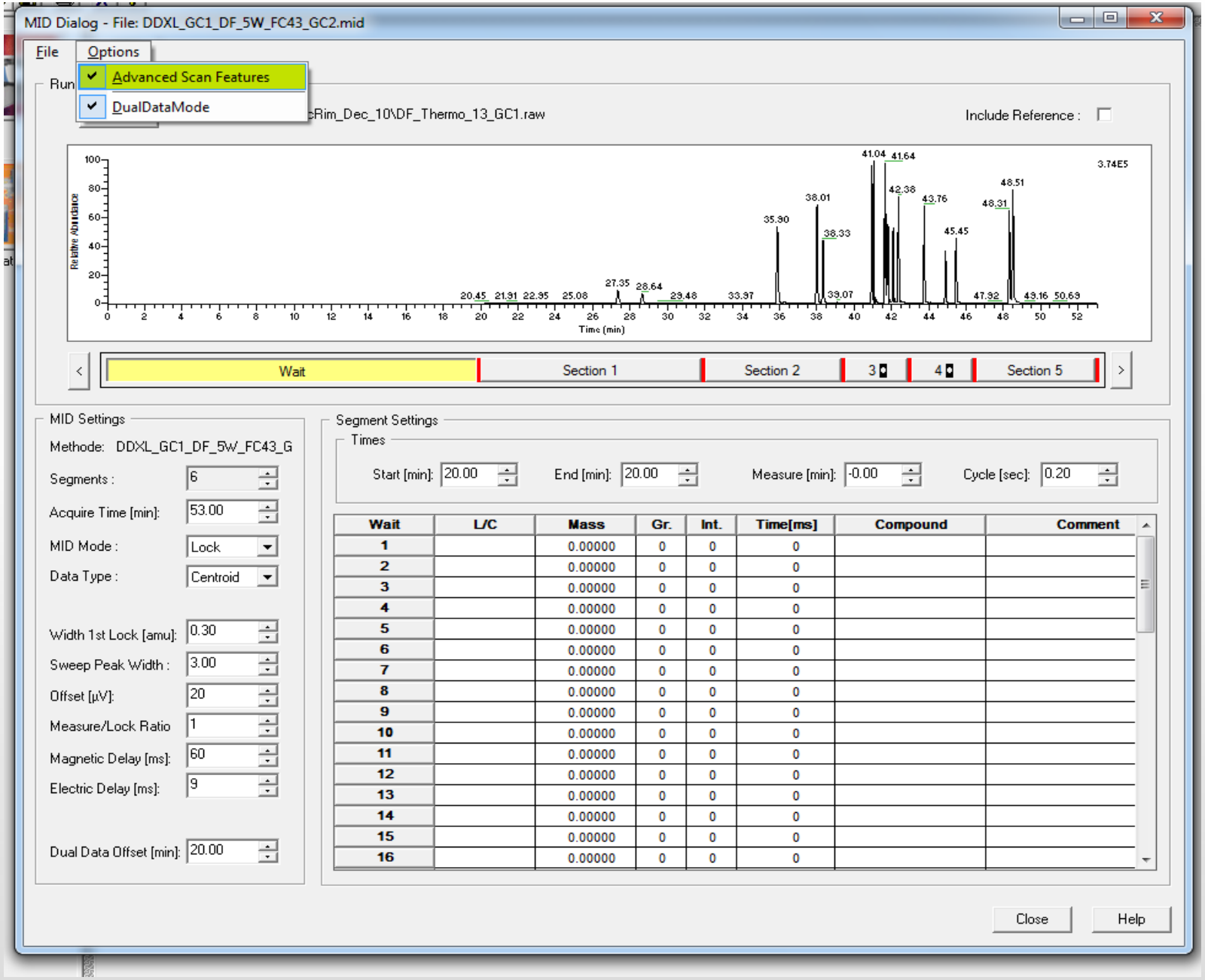


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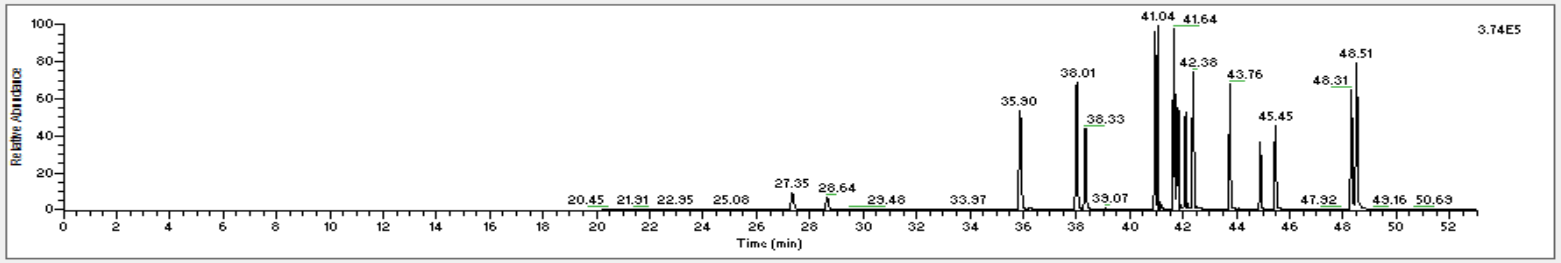
MID Dialog - File: DDXL_GC1_DF_5W_FC43_GC2.mid

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

Methode: 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 | Cali | 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

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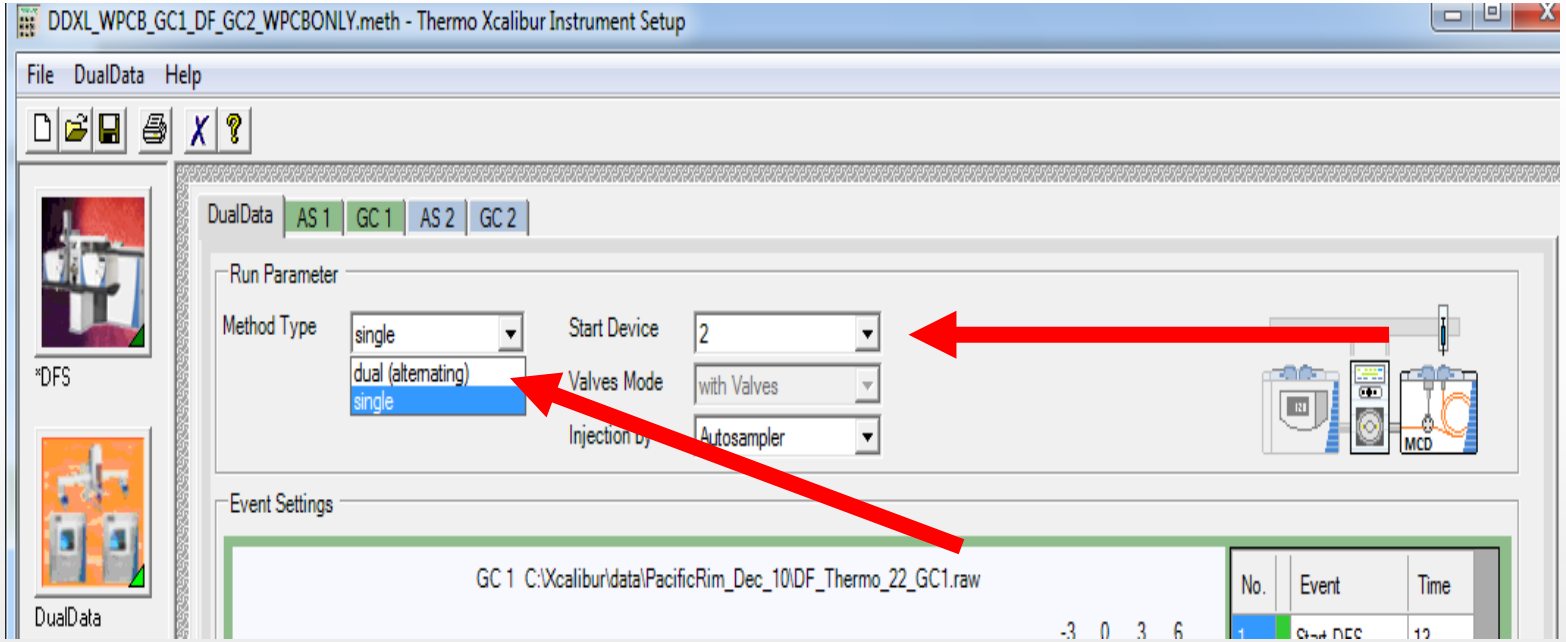


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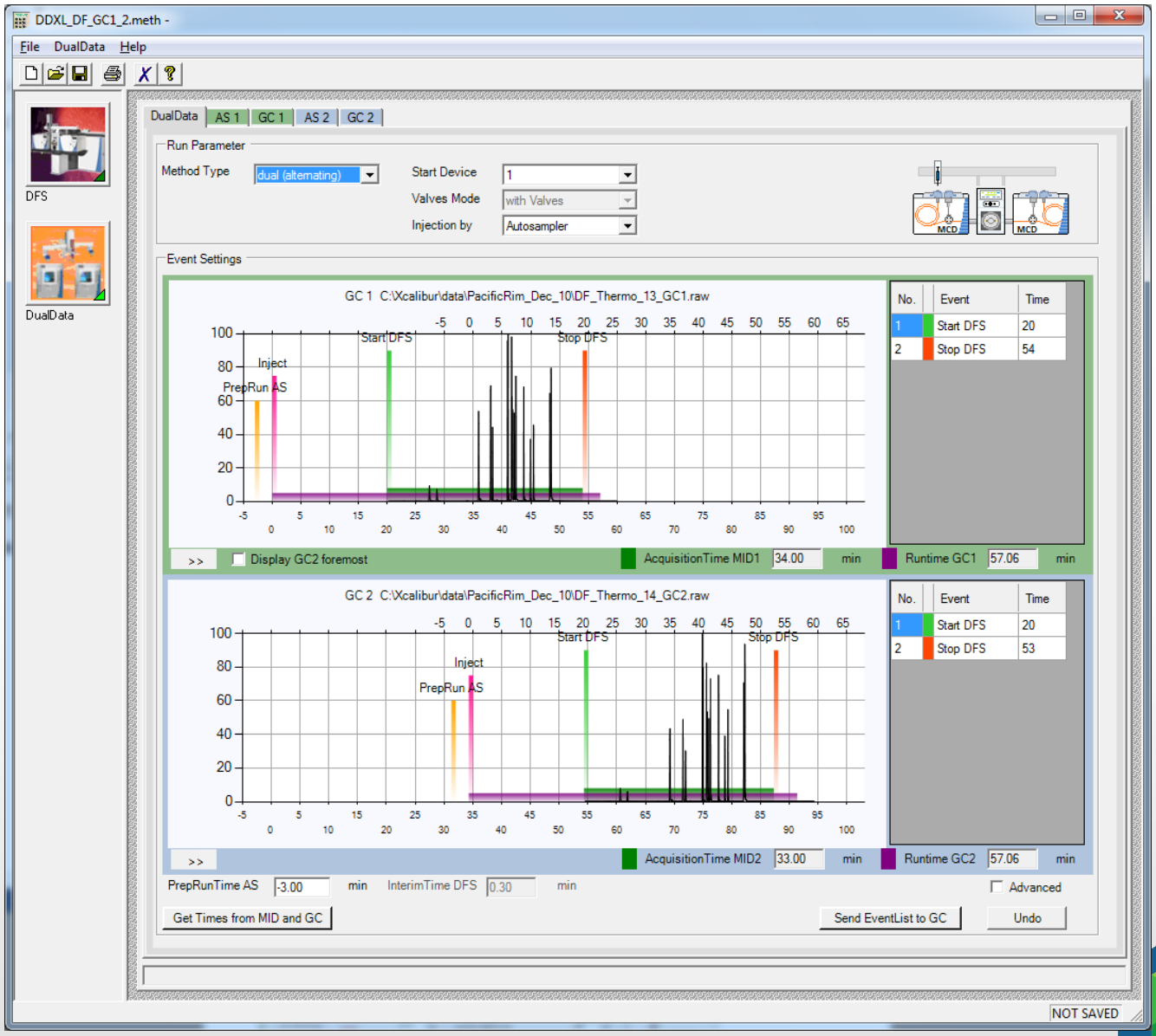
# Dual PCDD/F

Runtime DFS – 62 minutes or 23 inj/day

Runtime DualData XL – 67 minutes to complete cycle for both GCs

**42 injections in 24 h!**

82% more samples!

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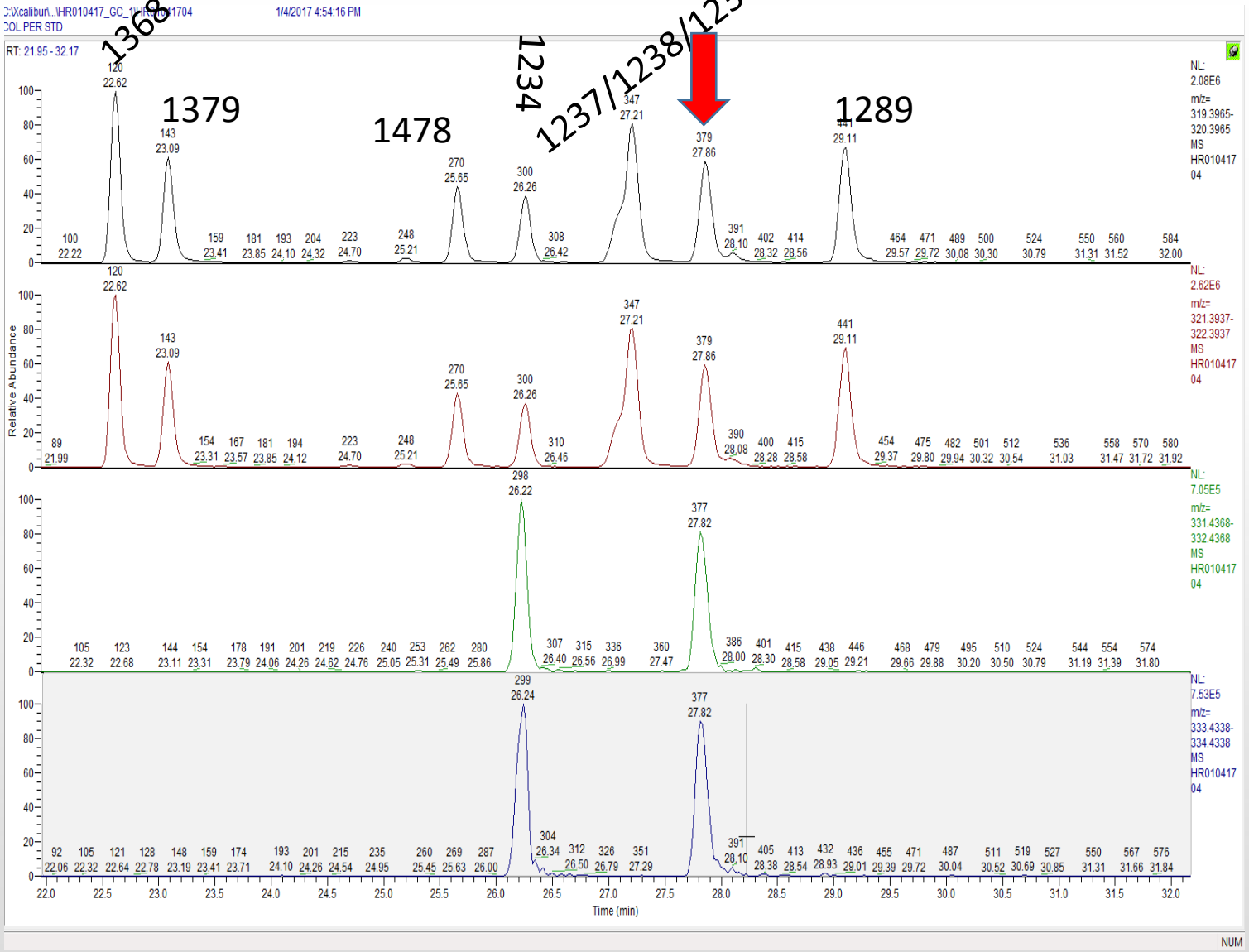
# Column Resolution - TCDD

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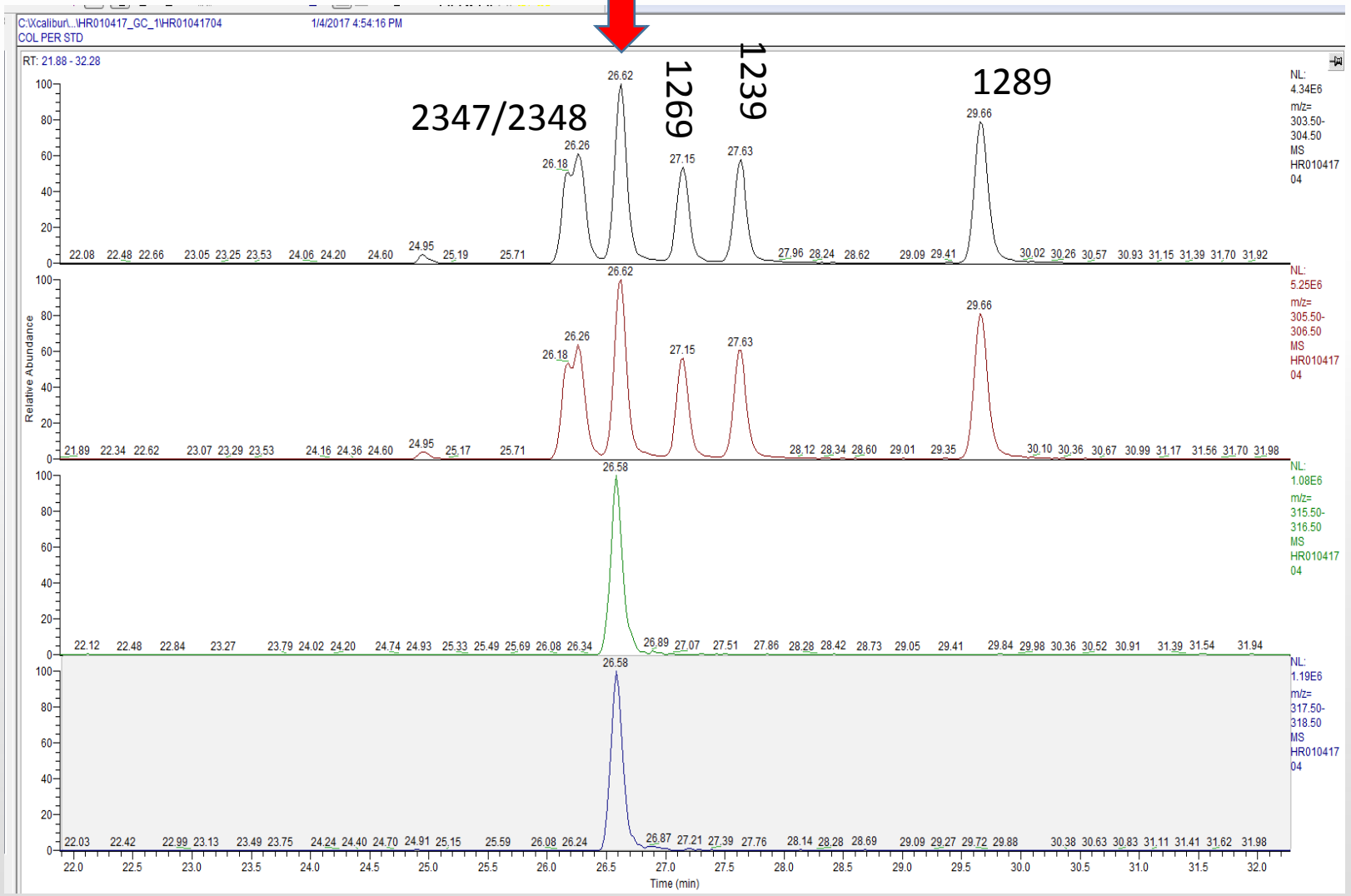
# Resolution - TCDF

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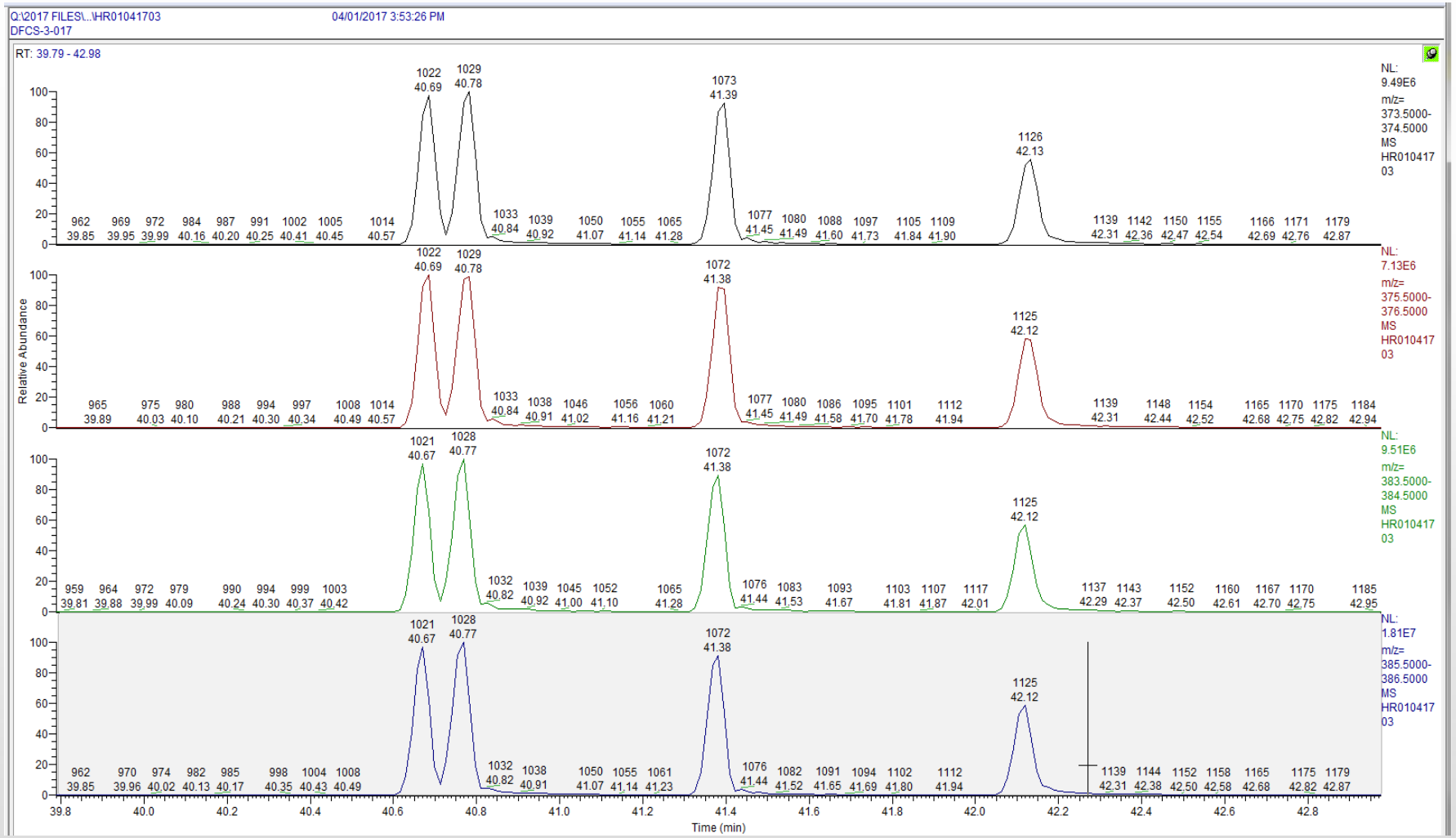
# HxCDF resolution

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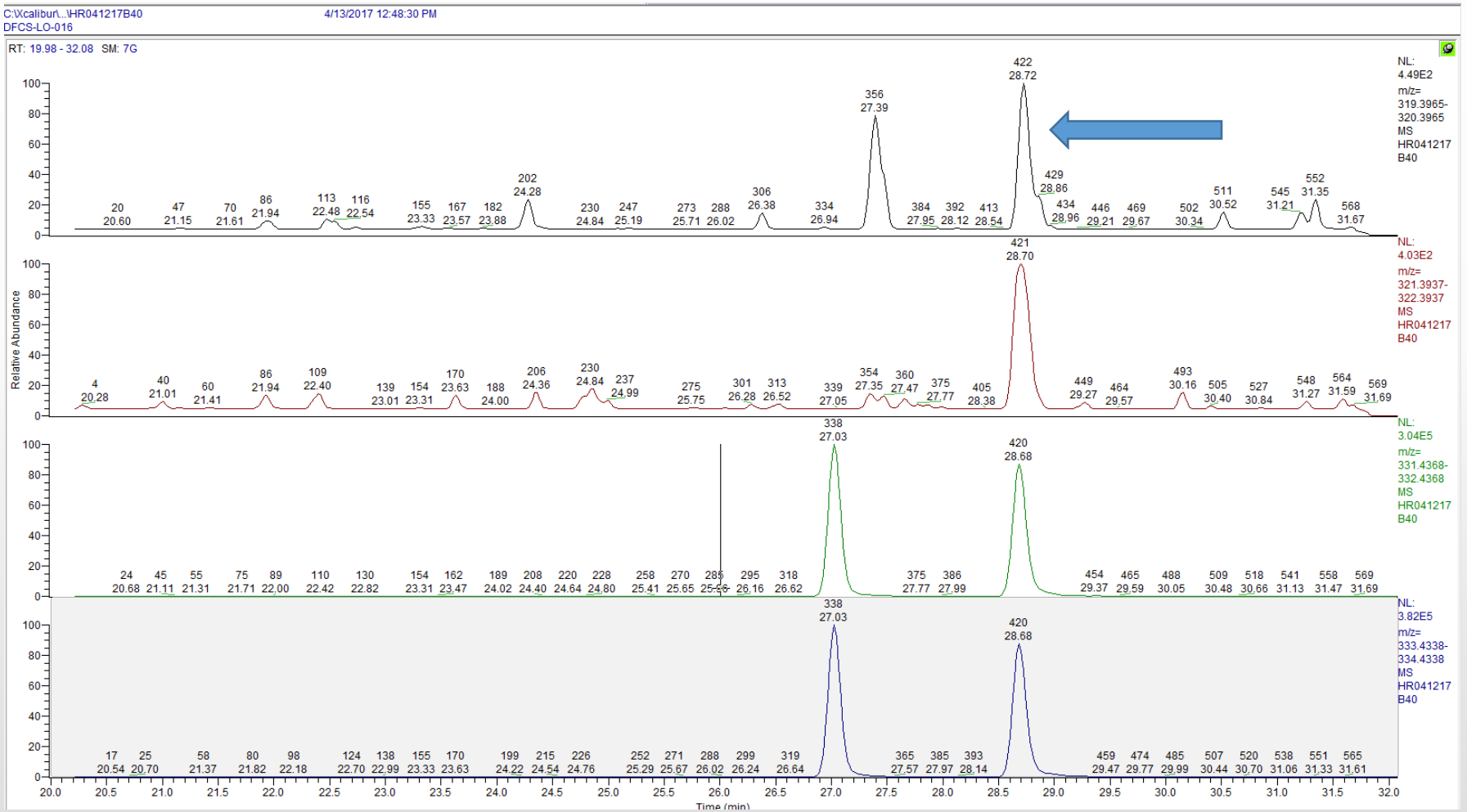
# TCDD - CS-Lo  0.1 pg injected

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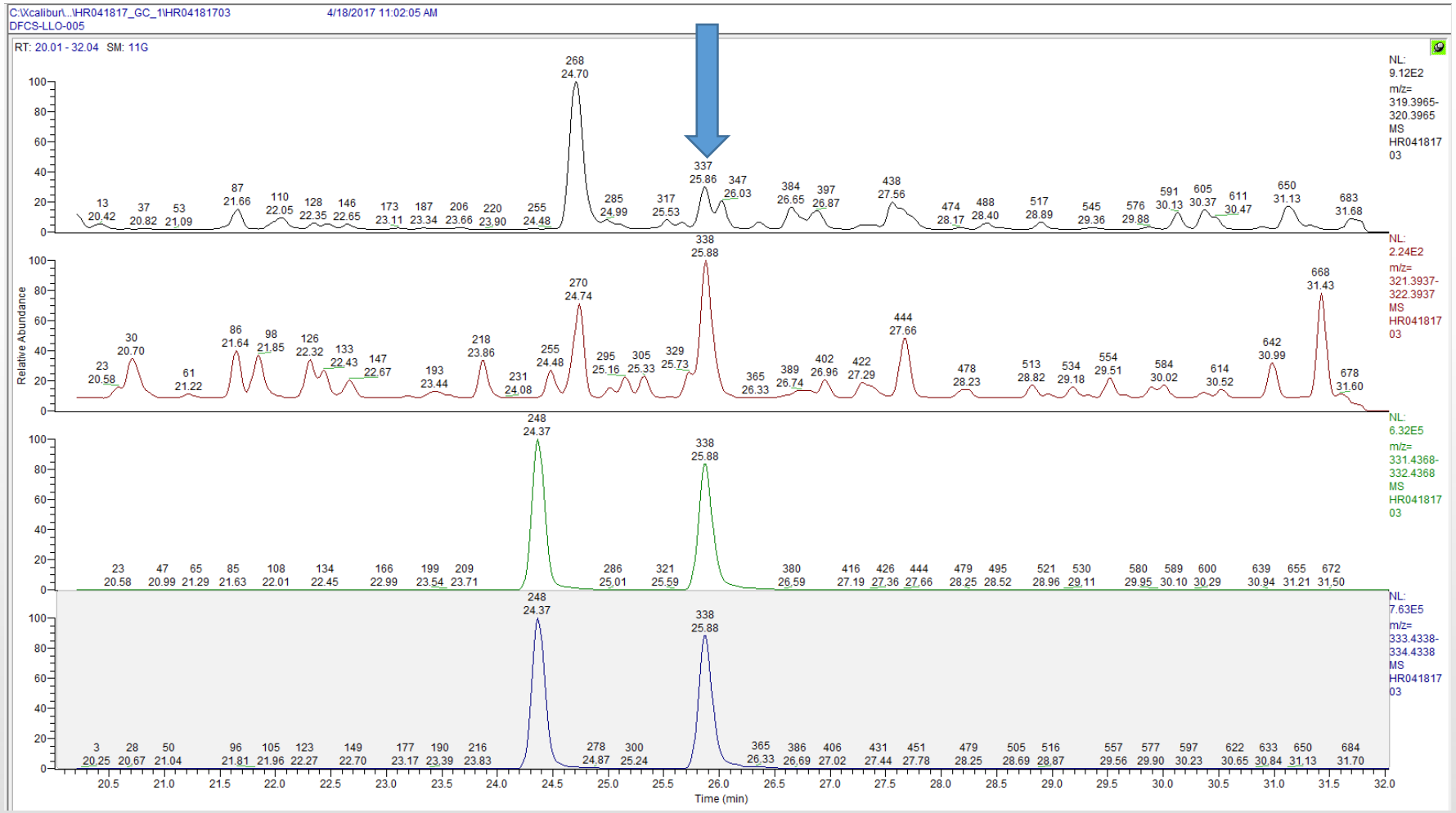
# TCDD – CS-LoLo!  20 fg injected

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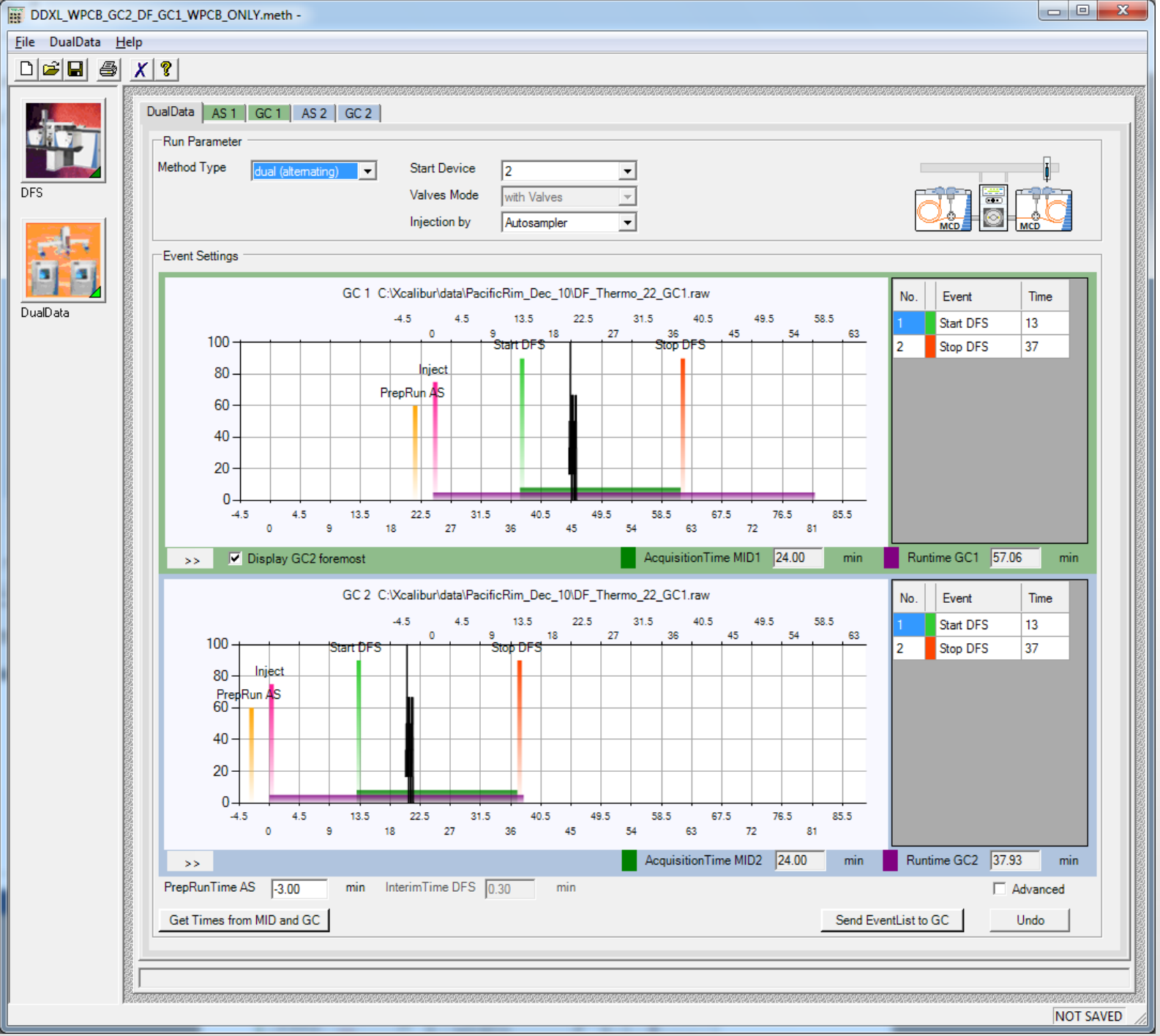


# Dual PCB

Runtime DFS – 68 minutes (21 inj/day)

Runtime DualData XL – for dioxin-like PCBs 74 minutes to complete cycle for both GCs

**38 inj/day**

82% more analyses

Runtime DualData XL – for 209 congener PCBs 94 minutes to complete cycle for both GCs

**30 inj/day**

43% more analyses

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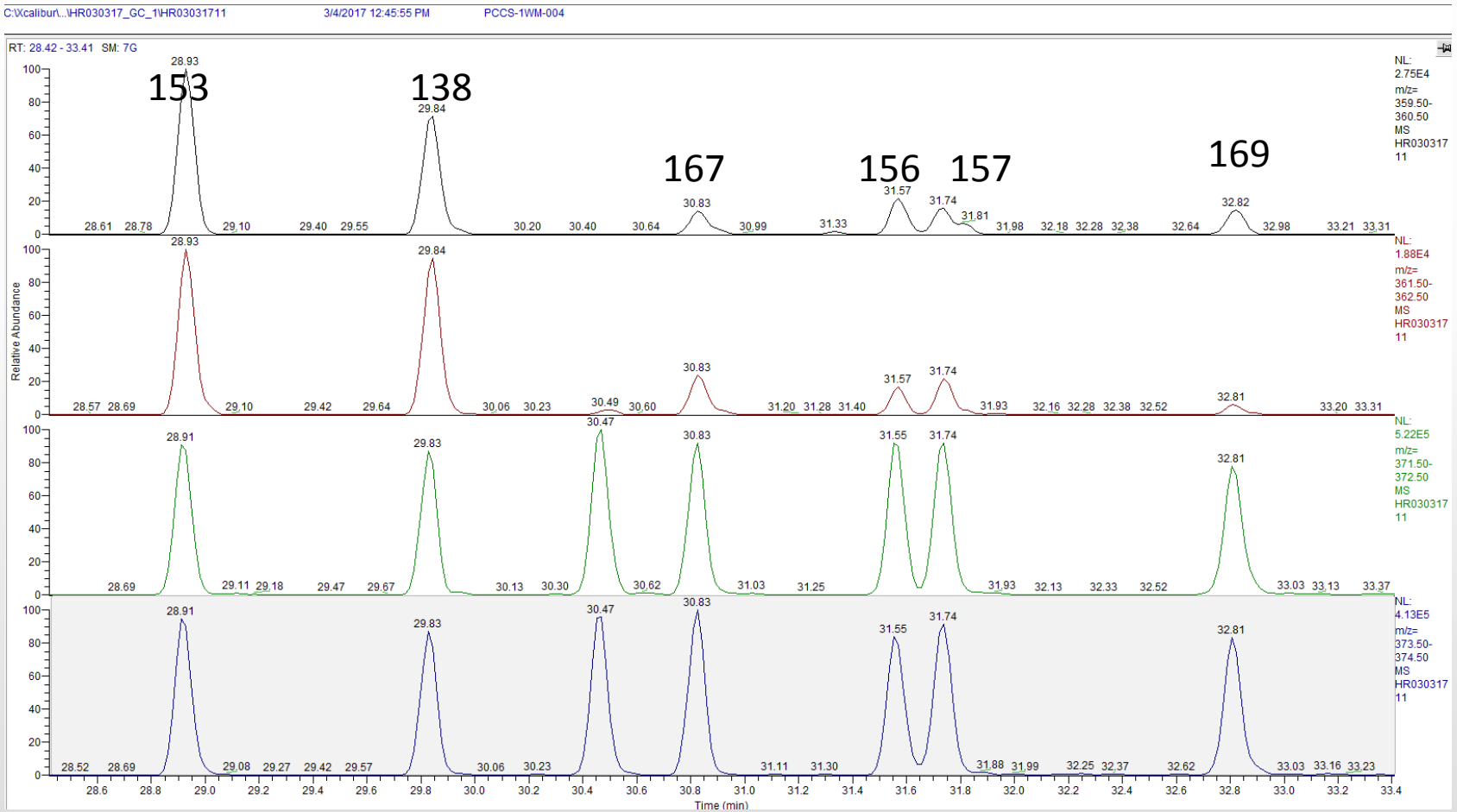
# HxCB @ 0.1/0.5 pg injected

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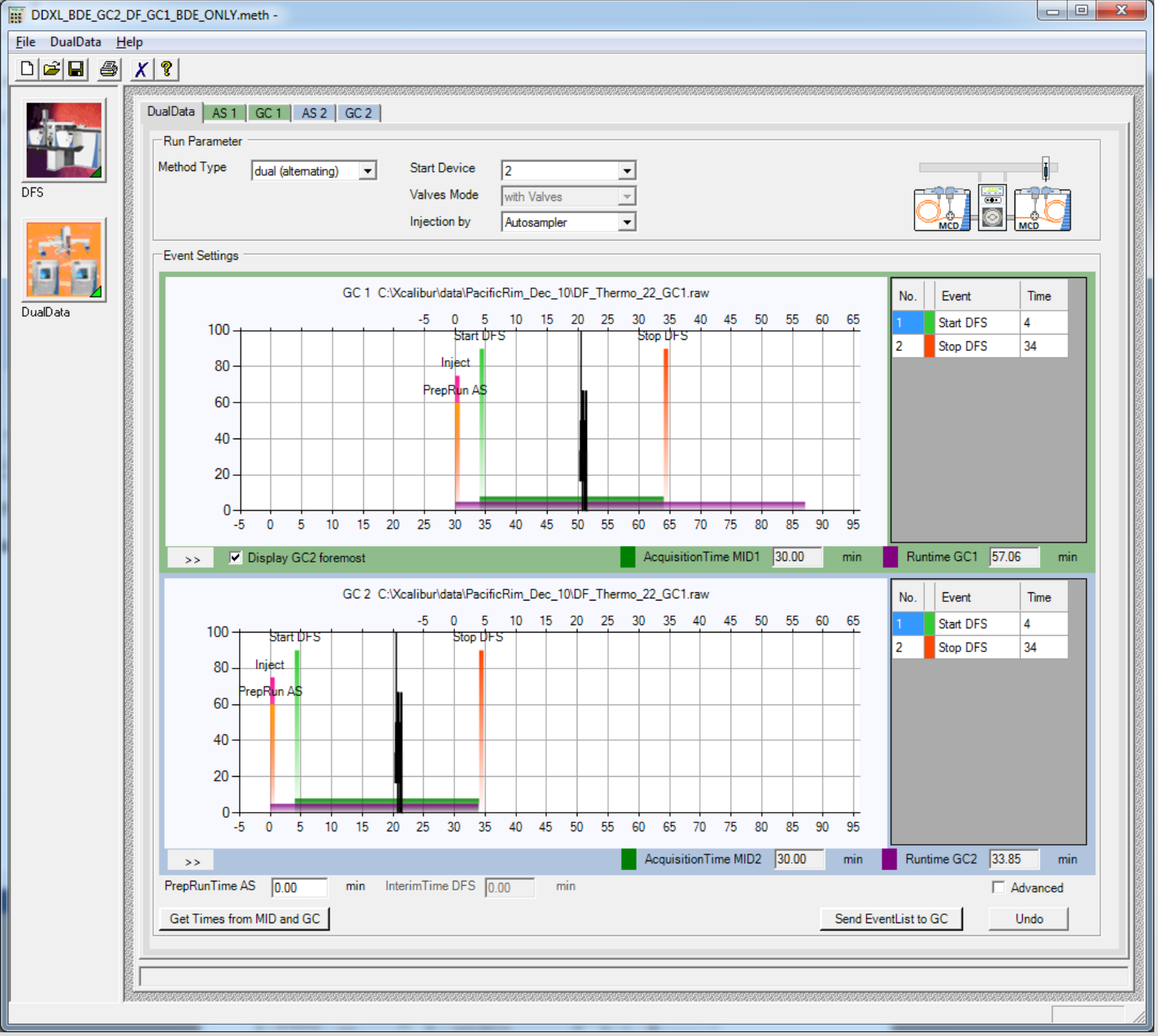


# Dual BDE

Runtime DFS – 41 minutes (35 inj/day)

Runtime DualData XL – 60 minutes to complete cycle for both GCs

**47 inj/day**

34% more runs!

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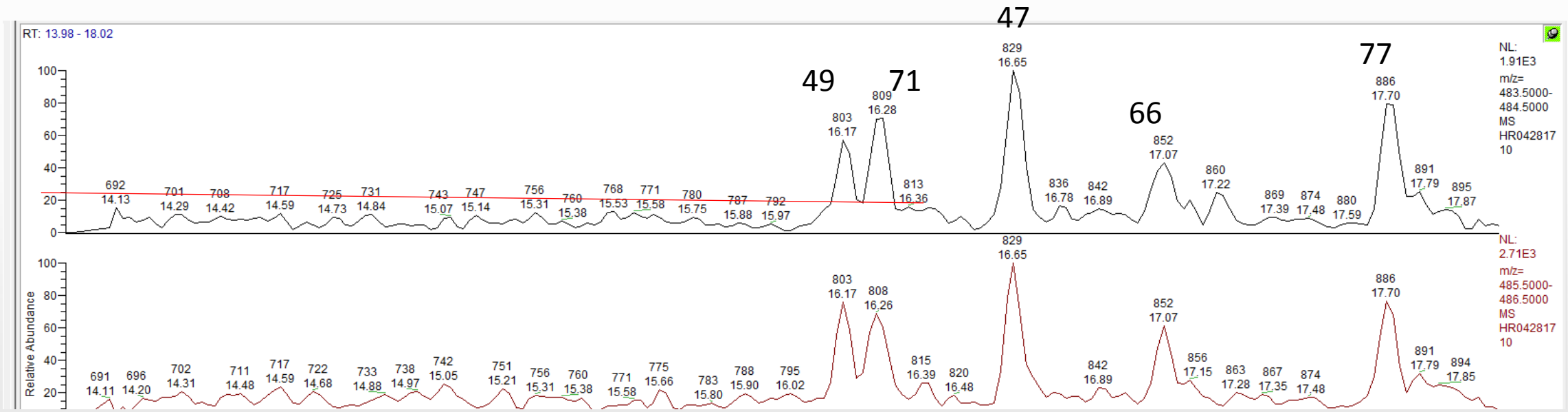
# TeBDE @ 0.5 pg injected

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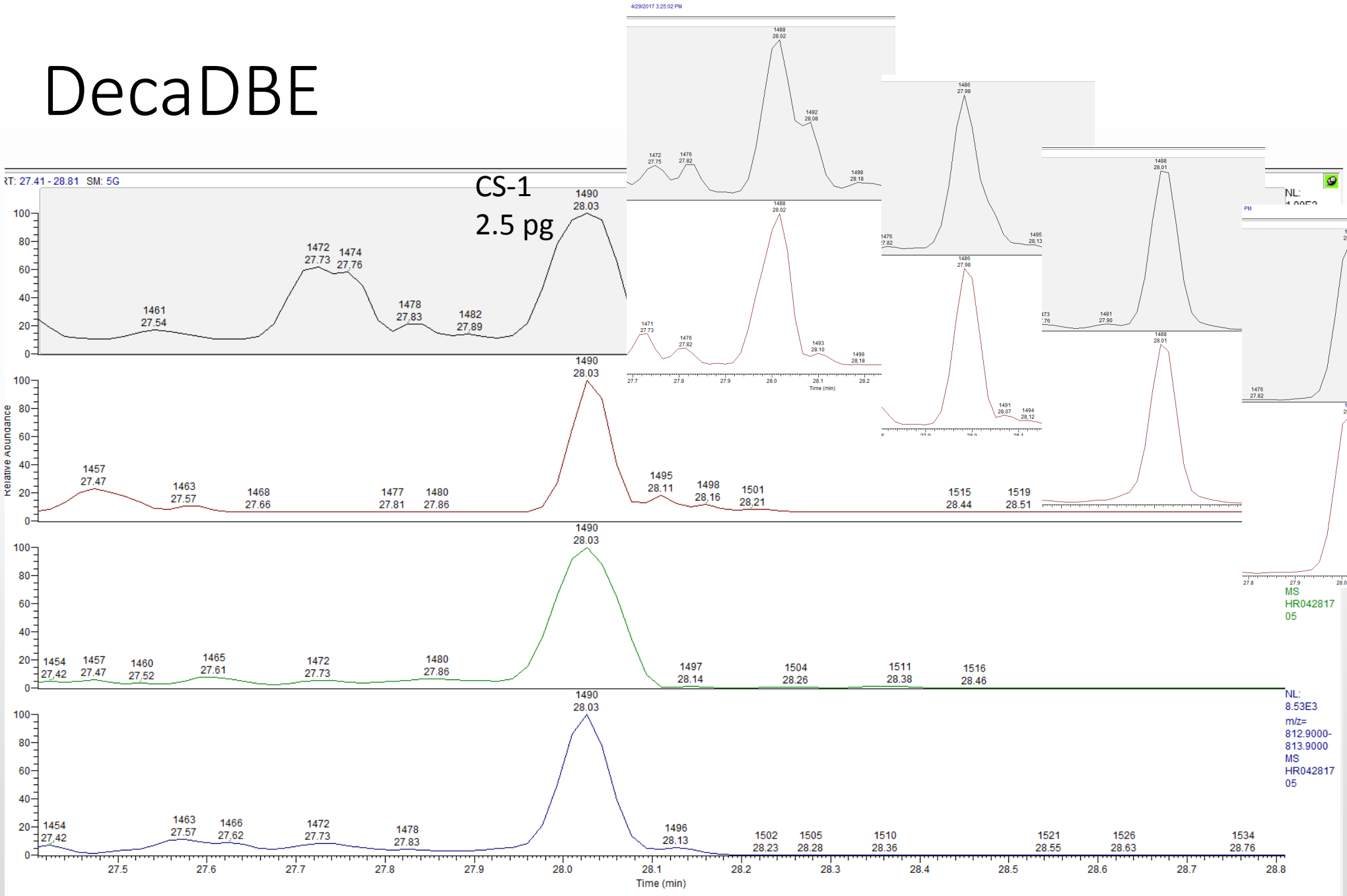
# DecaDBE

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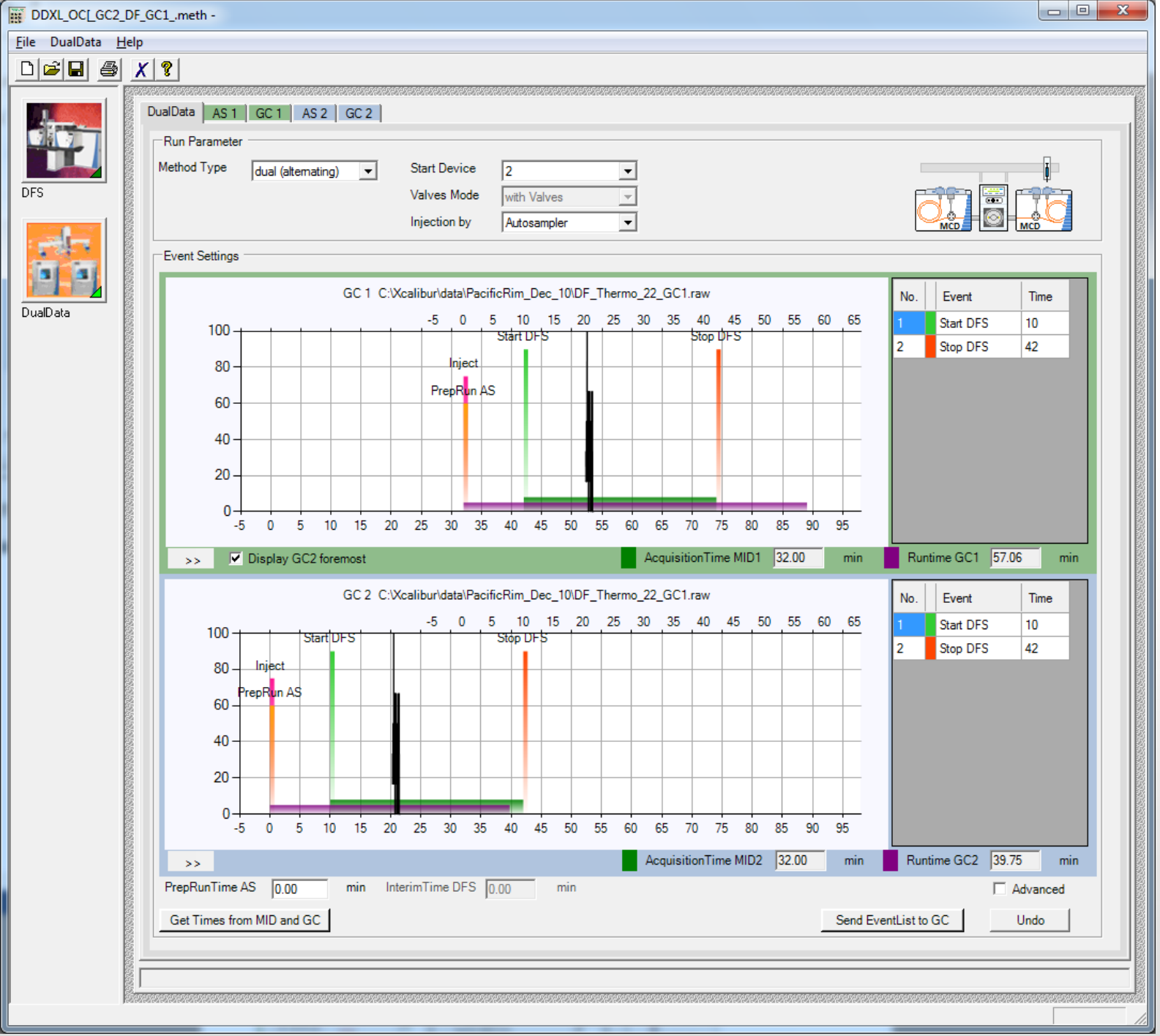


# Dual OCP

Runtime DFS – 51 minutes (28 inj/day)

Runtime DualData XL – 64 minutes to complete cycle for both GCs

**44 inj/day**

57% more analyses

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# 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

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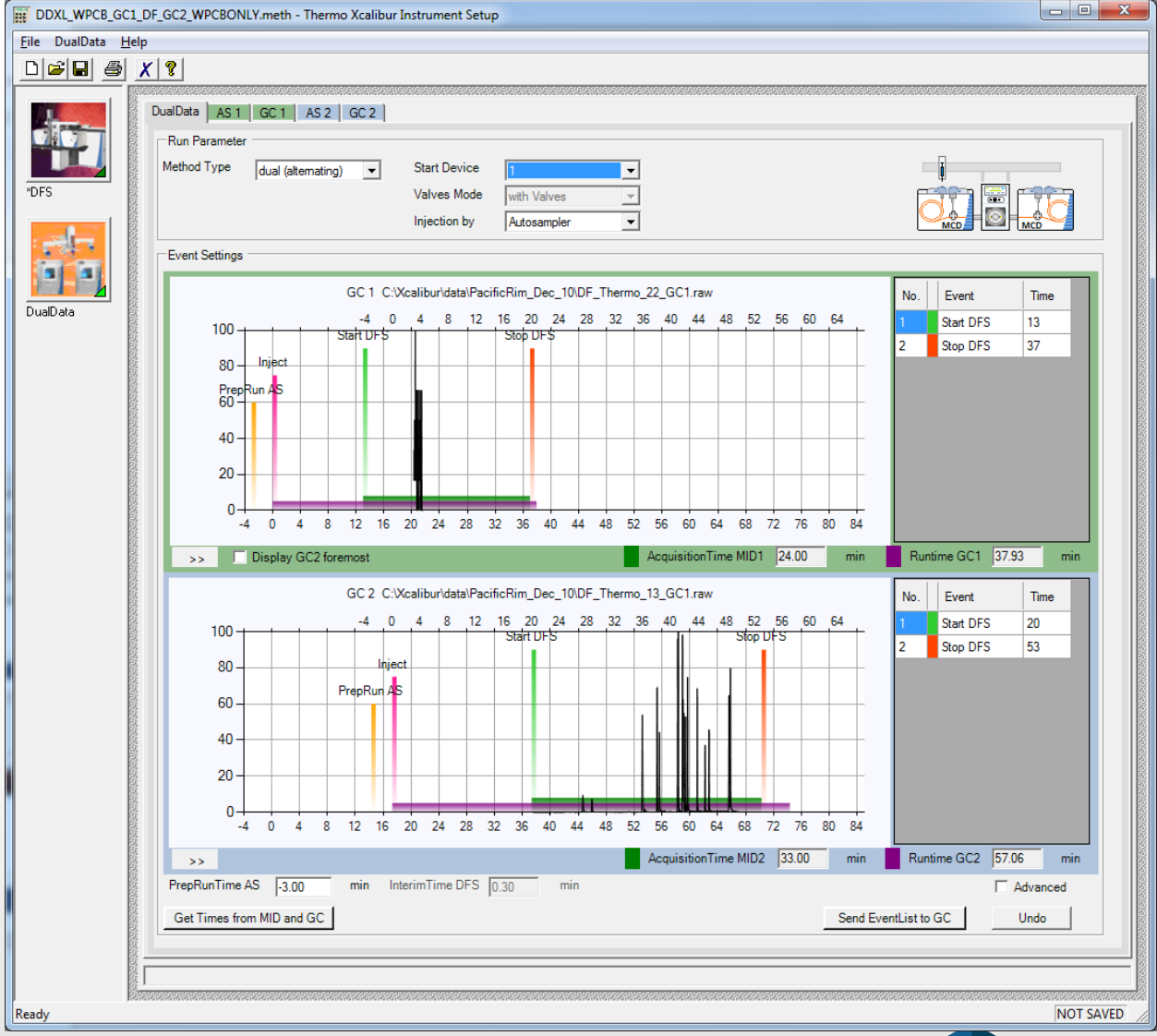
# PCDD/F & dlPCB

PCDD/F Runtime DFS – 62 minutes

PCB Runtime DFS – 48 minutes

Runtime DualData XL – 57 minutes to complete cycle for both GCs

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

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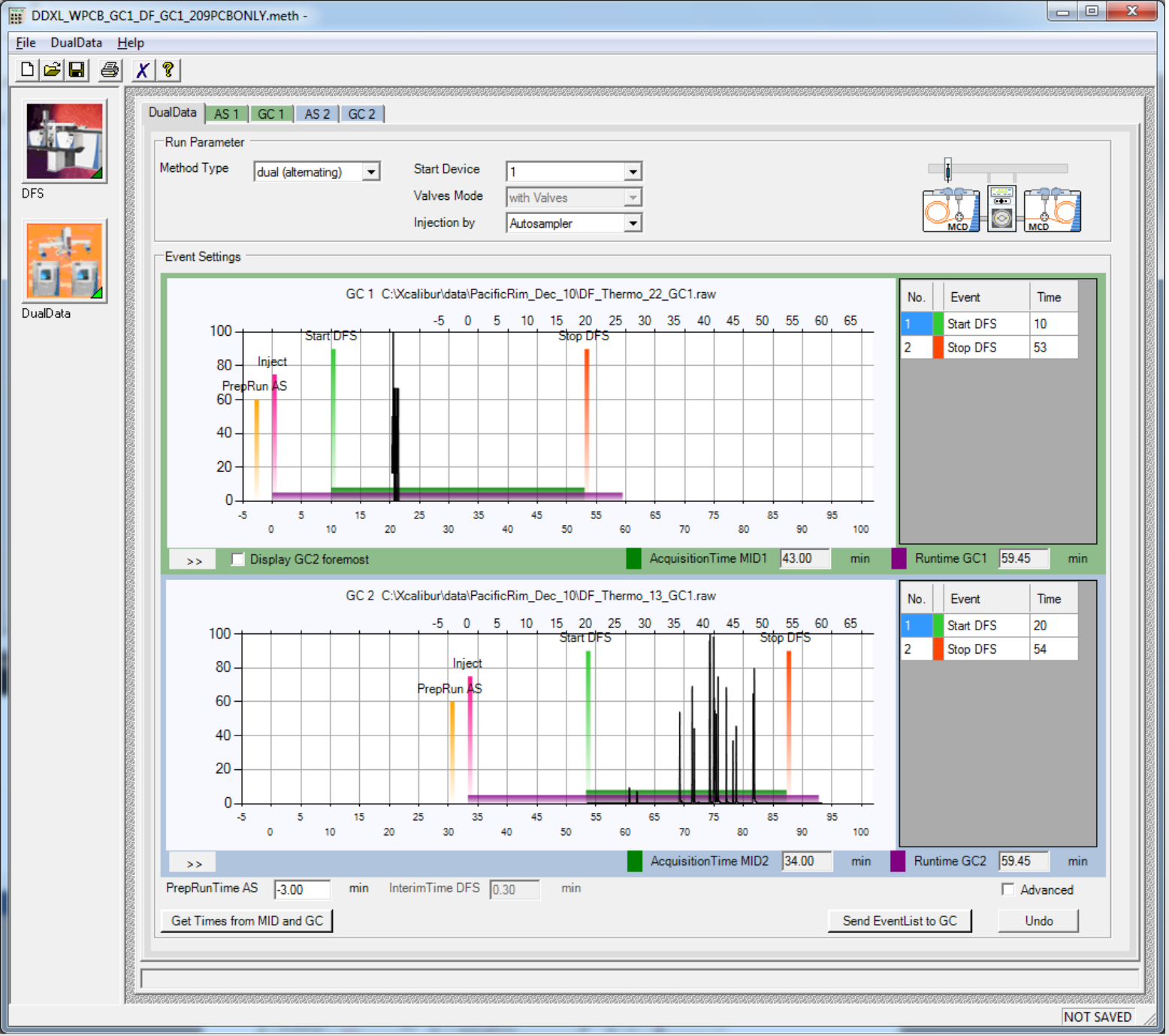


# PCDD/F and 209 congener PCB

PCDD/F Runtime DFS – 62 minutes

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

Runtime DualData XL – 77 minutes to complete cycle for both GCs

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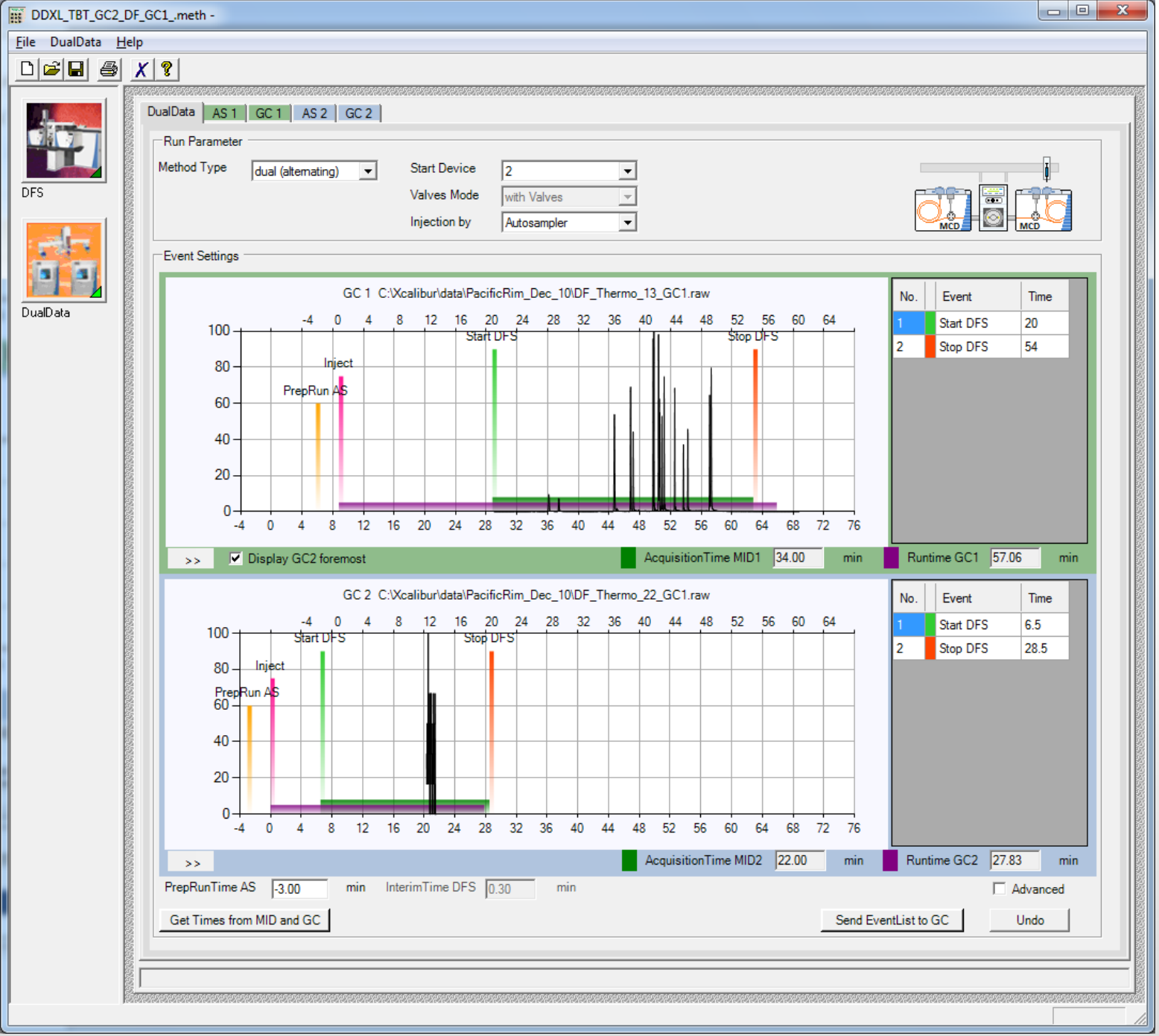


# PCDD/F & TBT

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!!

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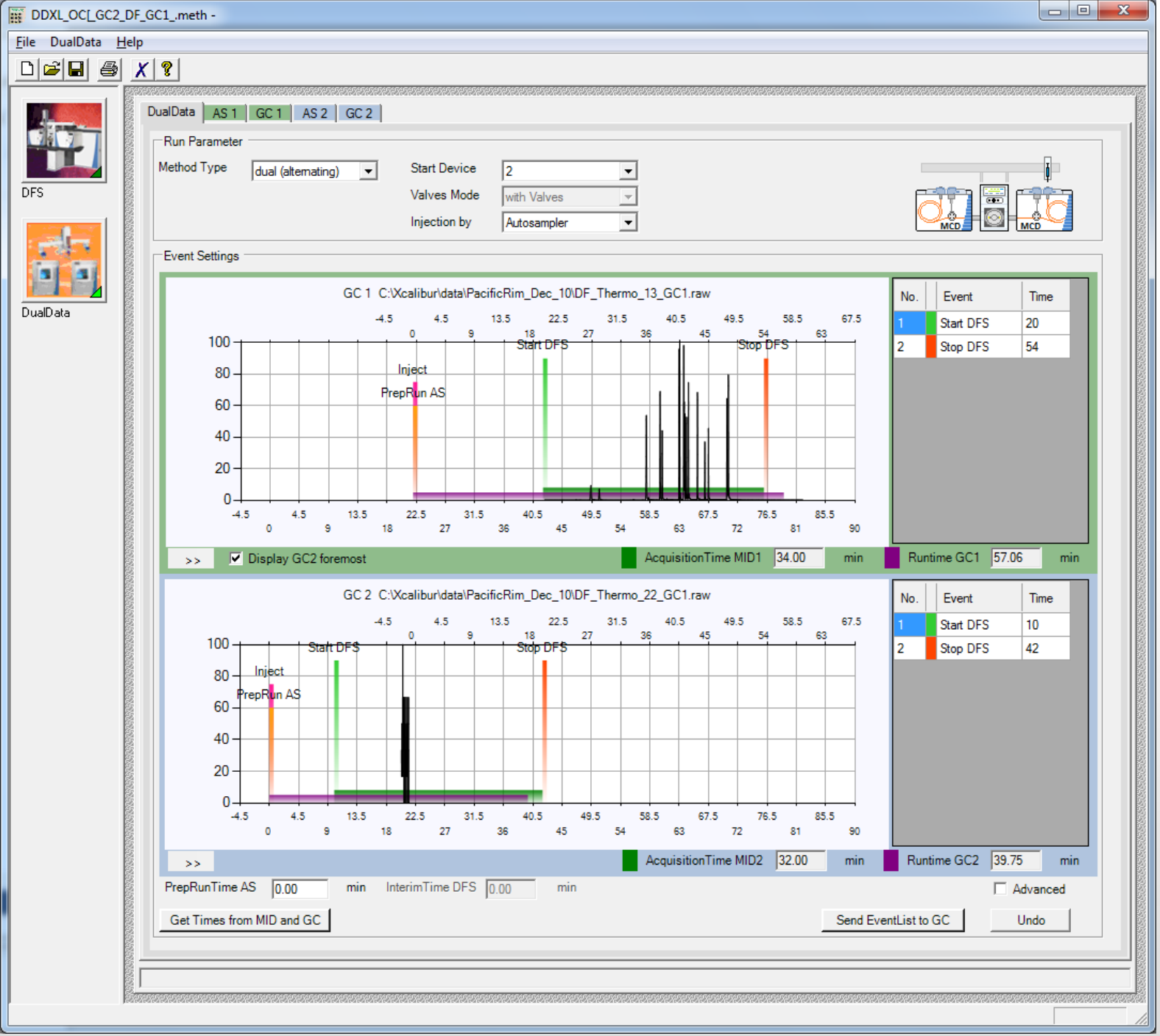


# PCDD/F & OCP

PCDD/F Runtime DFS – 62 minutes

OCP Runtime DFS – 51 minutes

Runtime DualData XL – 66 minutes

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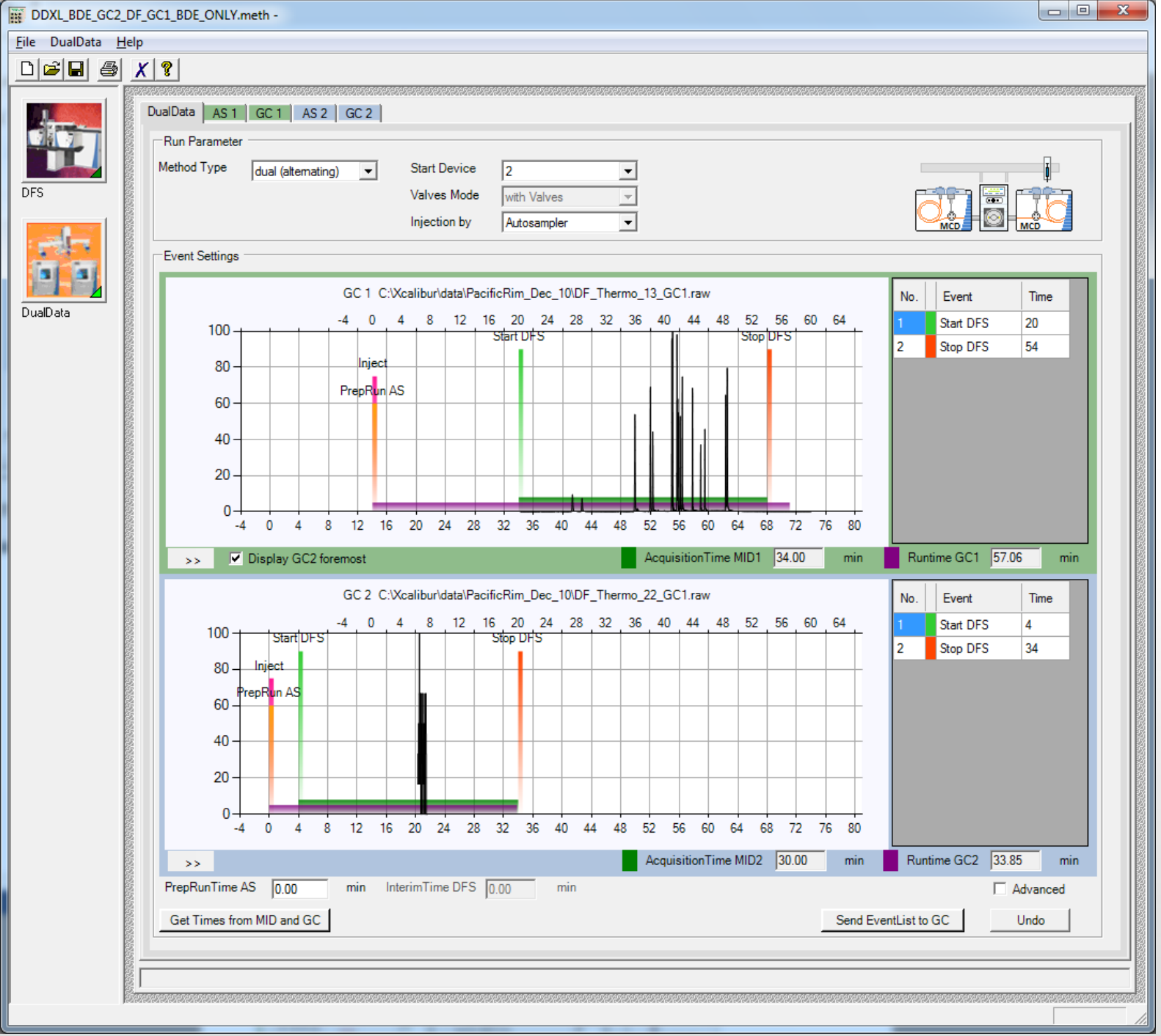


# PCDD/F and PBDE

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.

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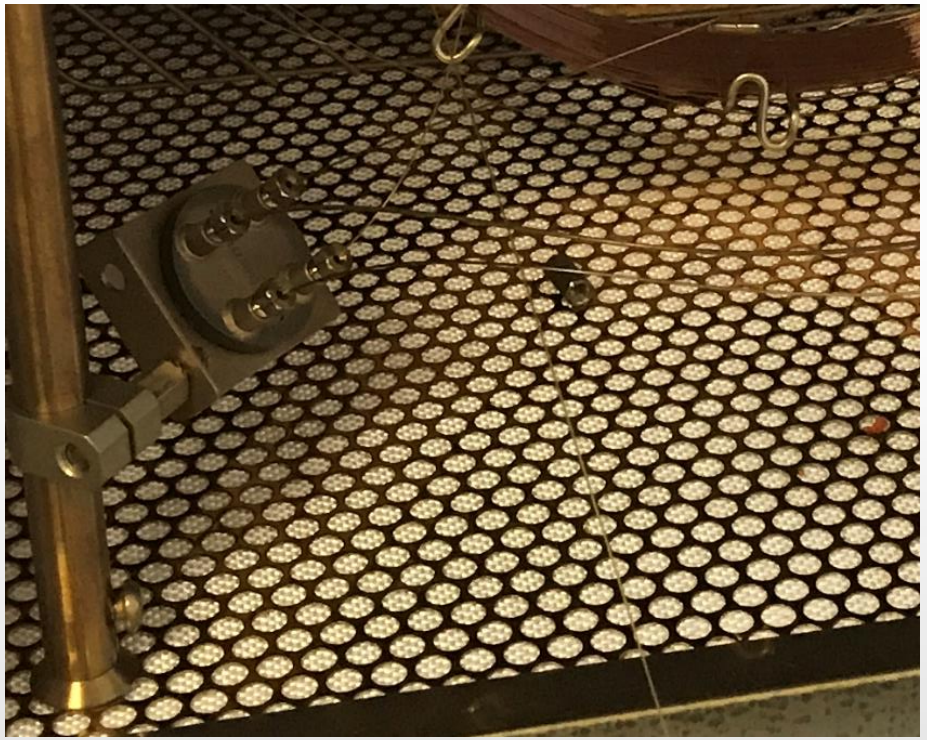
# Conclusions

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



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# Thank you from Pacific Rim Labs.


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