



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

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



My Business Partner and co-founder



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



VG70 arrives!



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Beginnings

Dioxin 2005 - Toronto



Thermo Fisher Scientific 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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Scientific Research and Experimental Development

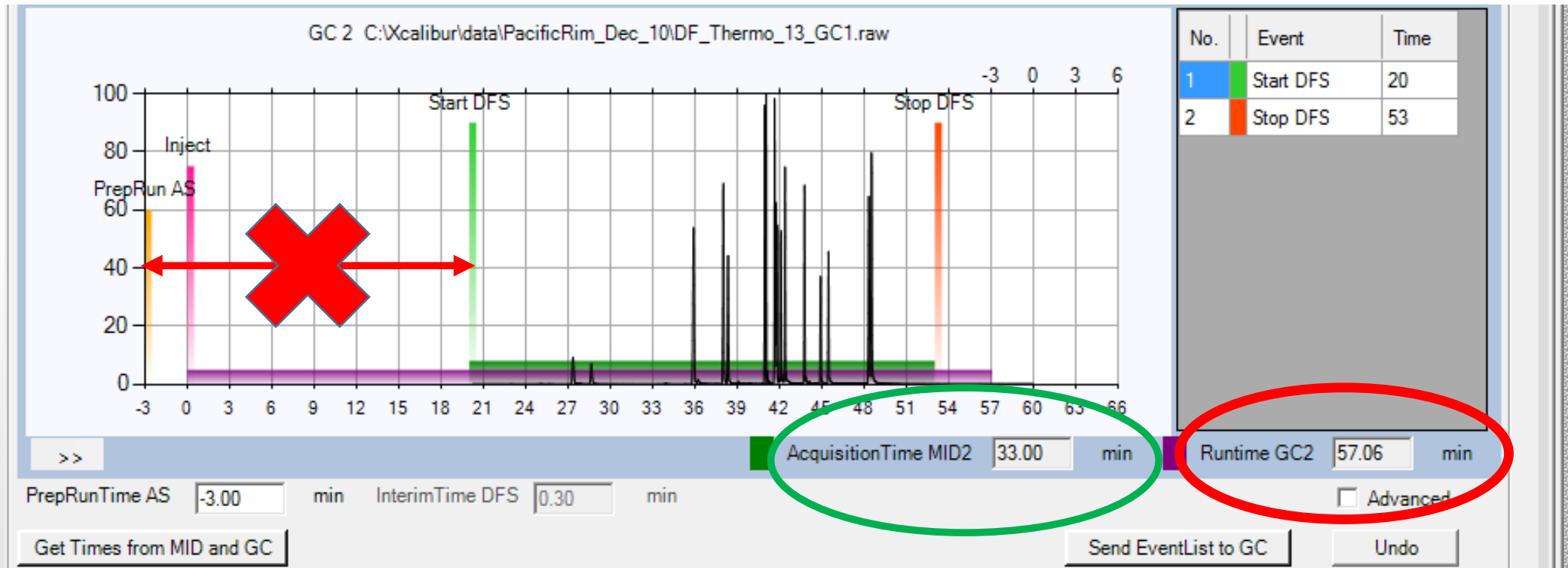
- We thrive on innovation
 - PBDE method in 2005
 - 209 congener PCBs in 2005
 - Sub-ppb PAH analysis food in 2006
 - Published 2009 congener PCB by SGE HT8 column (2009)
 - Cape Tech column clean-up (2012)
 - OCPs by HRMS (2012)
 - Improved clean-up methods for dioxins/PCB (2014)
 - Rocket evaporator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

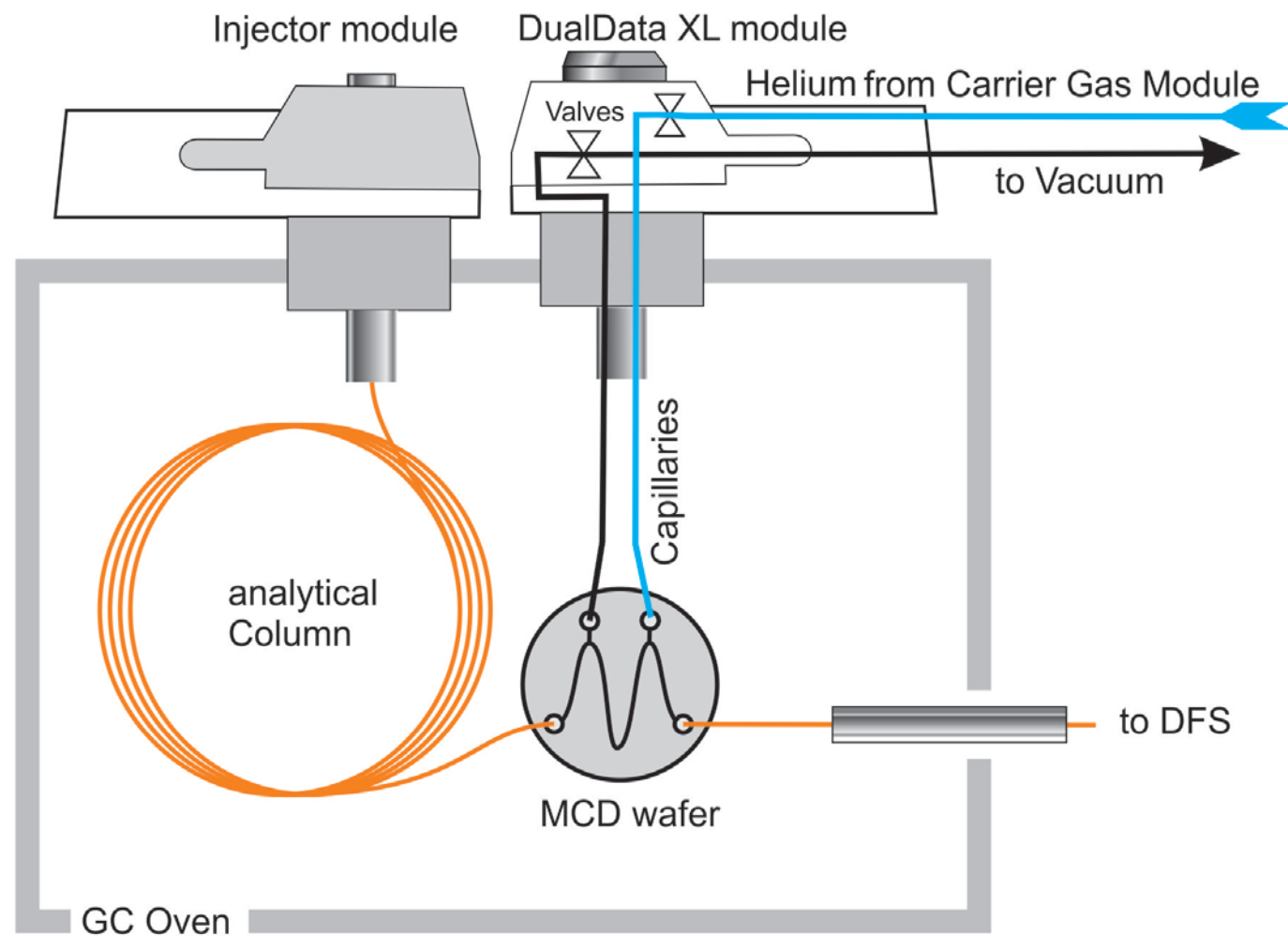


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What is Dual Data? PCDD/F analysis

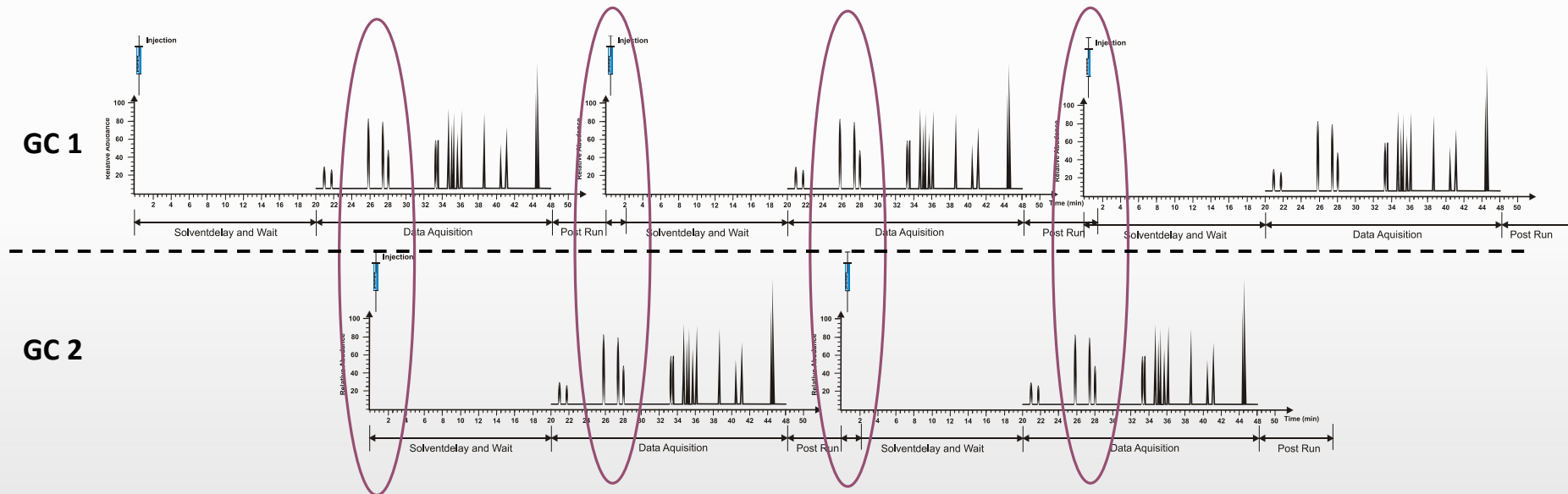
EPA 1613b – TCDD must elute >25 minutes



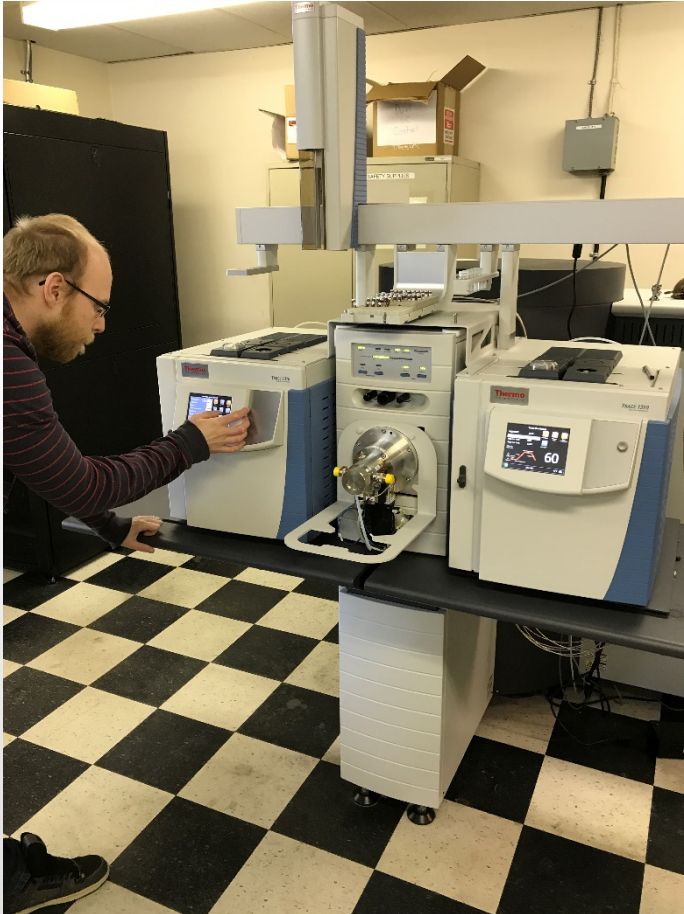


DFS DualData XL: Staggered Injection

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



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

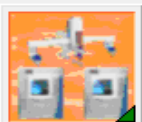
- DFS with dual 1310 GCs
- Older DFS can be converted, but cannot use Trace GCs.
- Will add a 6-way valve to control gases
- A gas module is installed next to your injector.
- New software



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*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

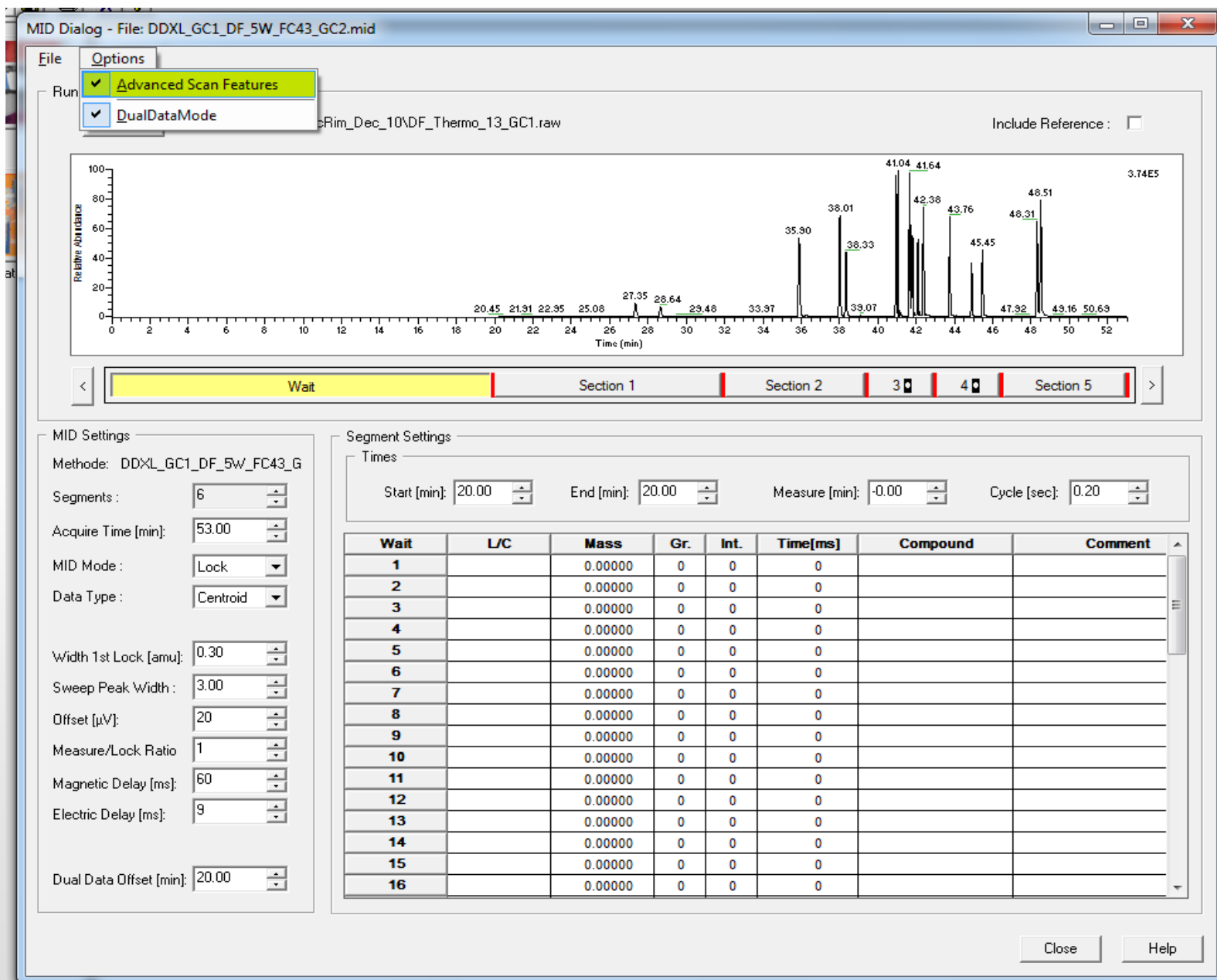
8000.00

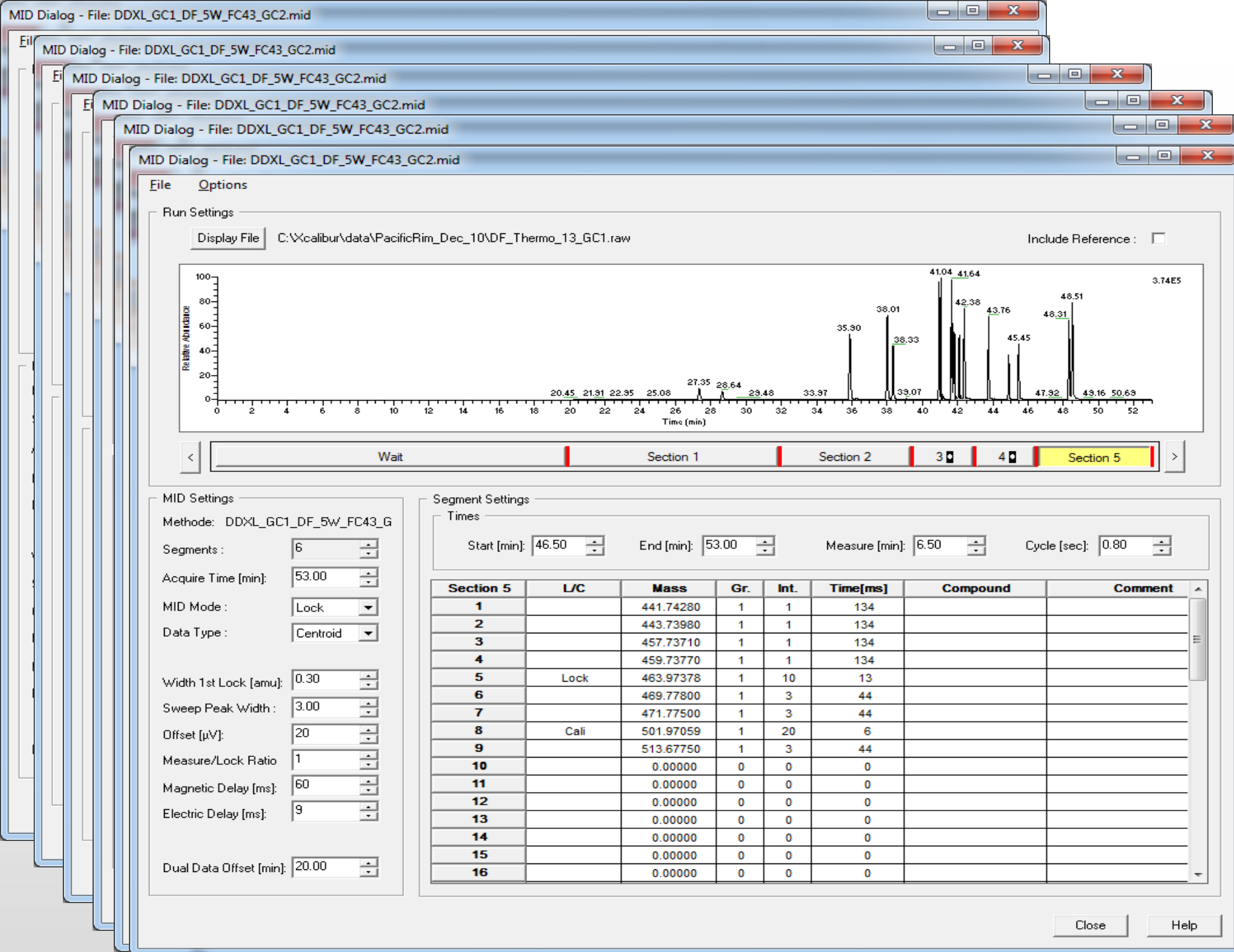
☒ Stop Sequence on Error

Lock Peak Mode: No Check

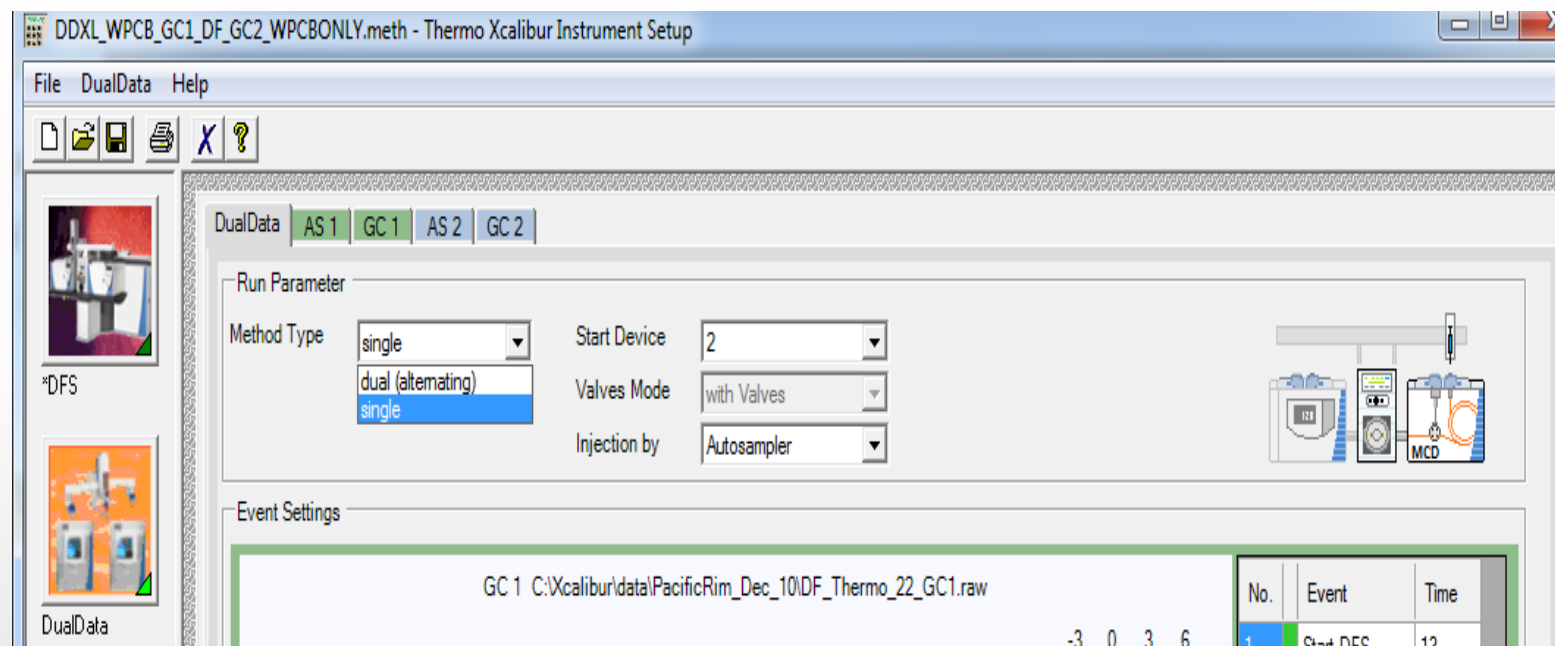


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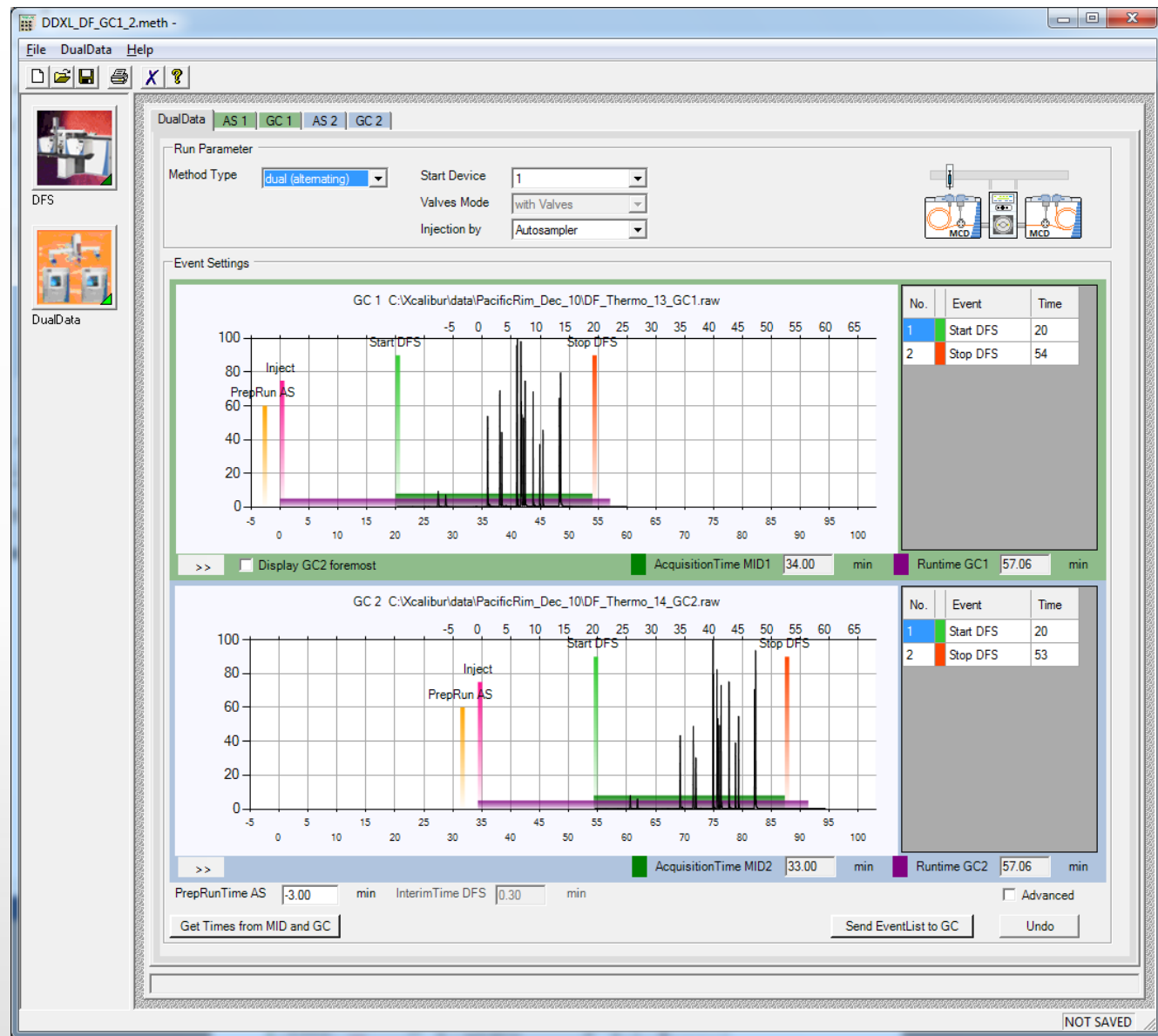
Dual PCDD/F

Runtime DFS – 62 minutes or 23 inj/day

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

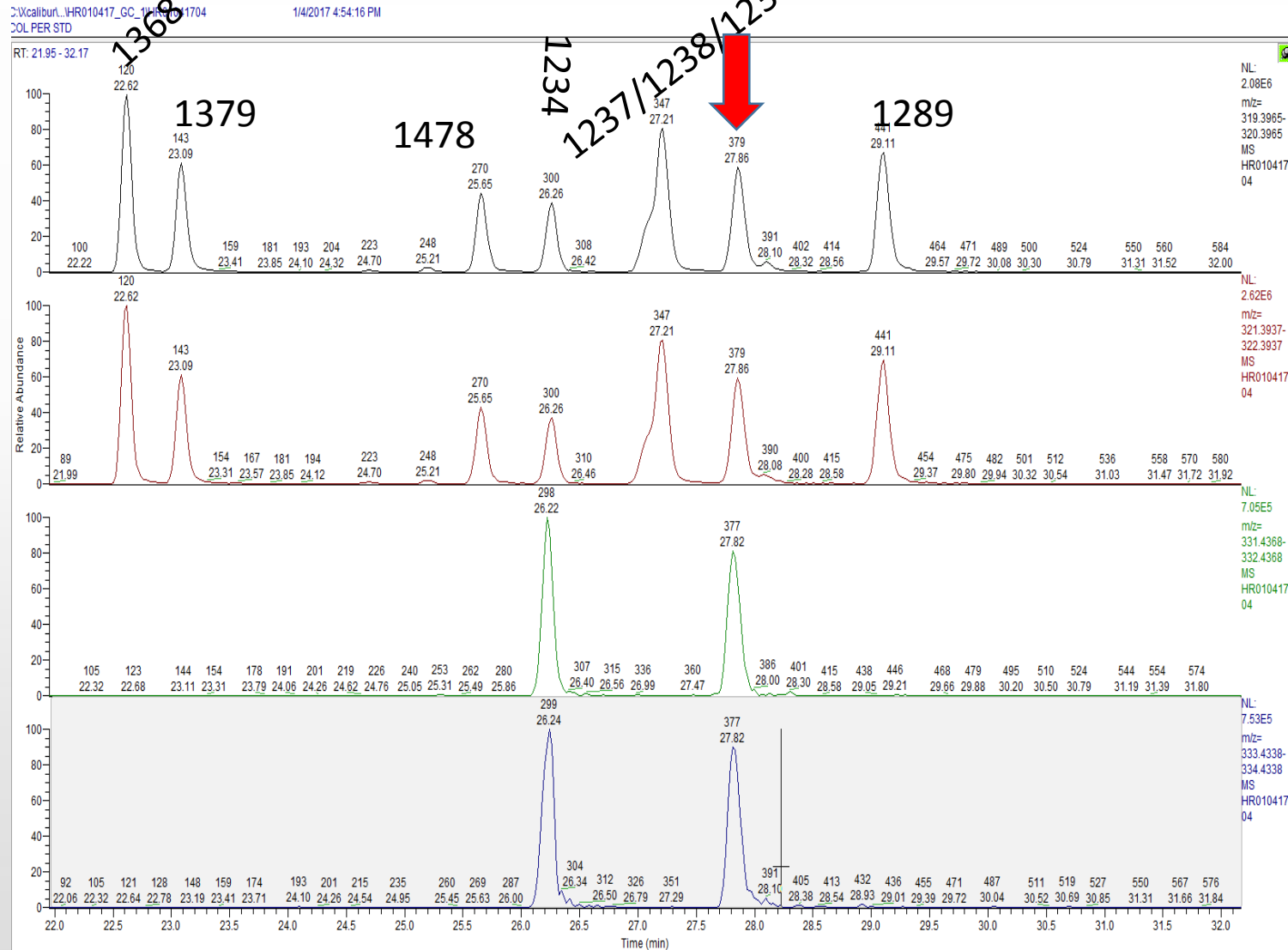
42 injections in 24 h!

82% more samples!



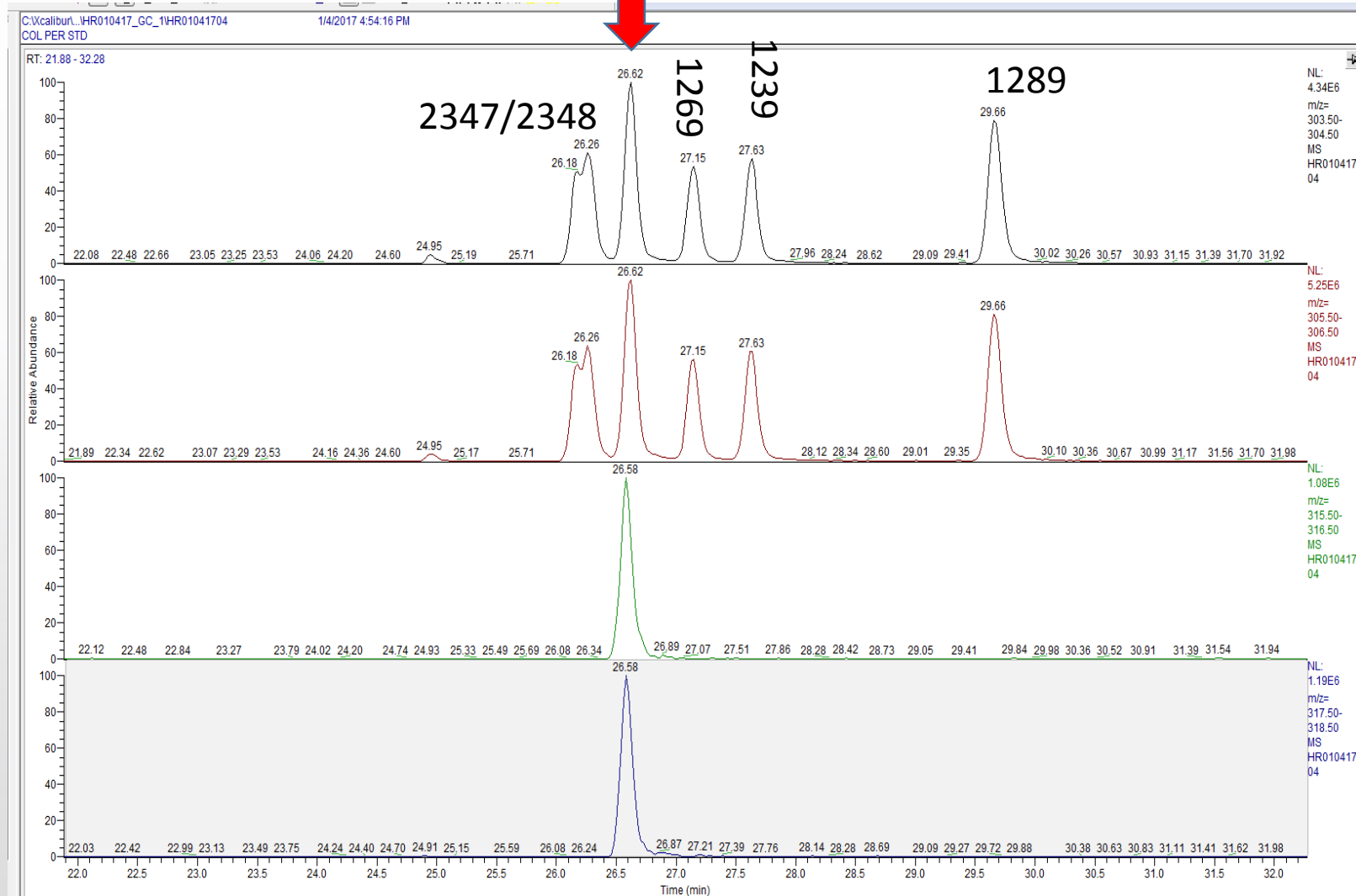
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Column Resolution - TCDD



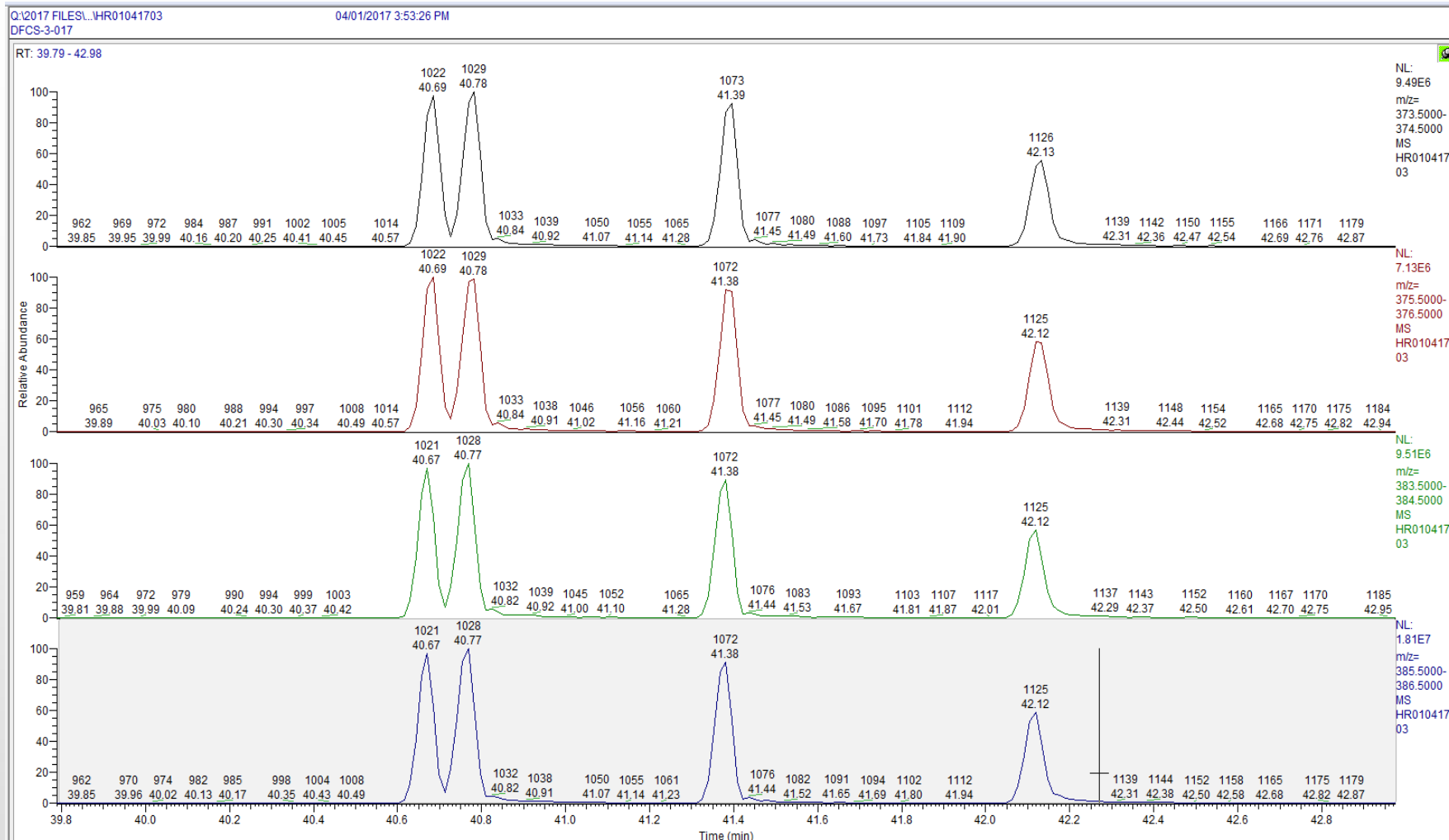
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Resolution - TCDF



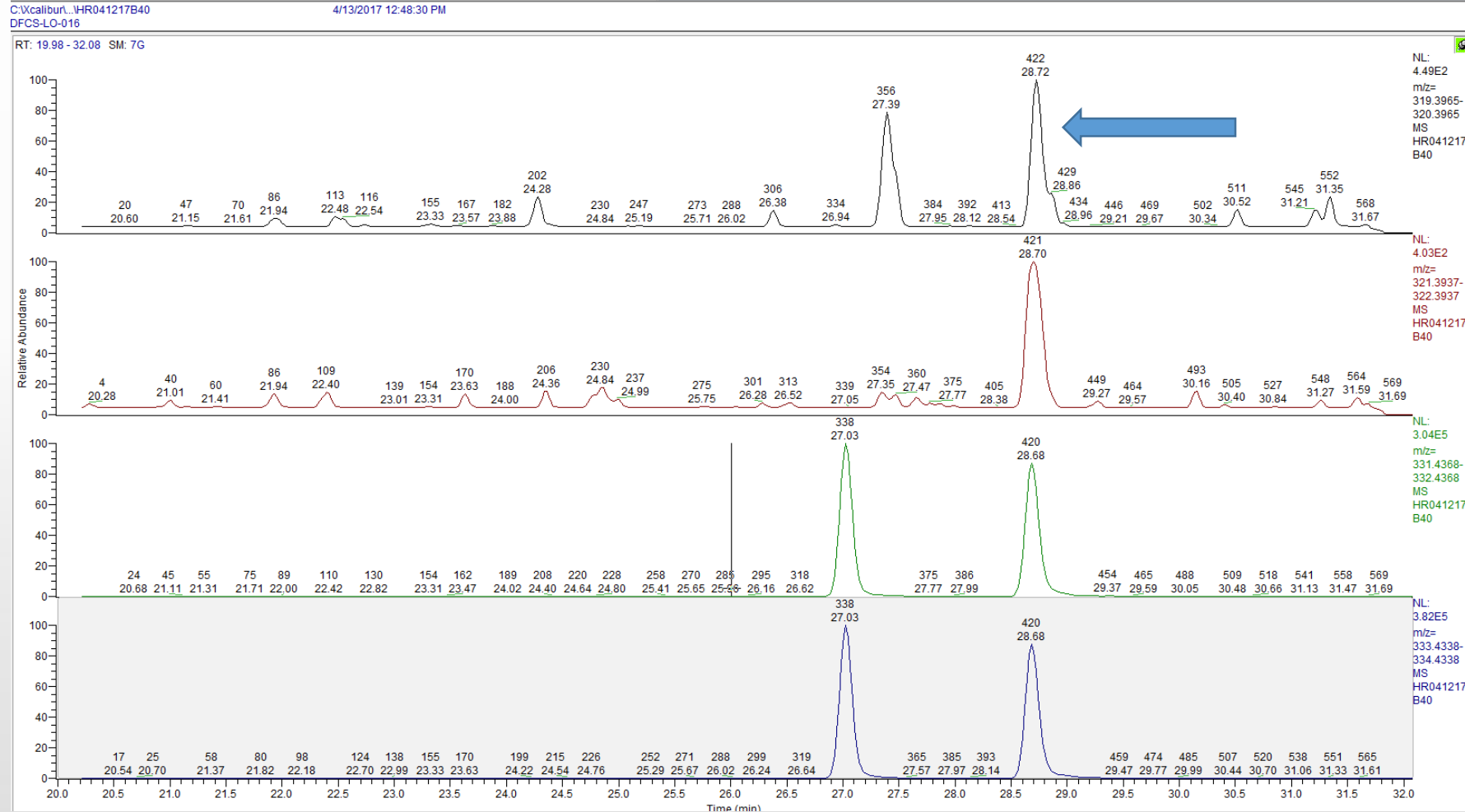
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HxCDF resolution

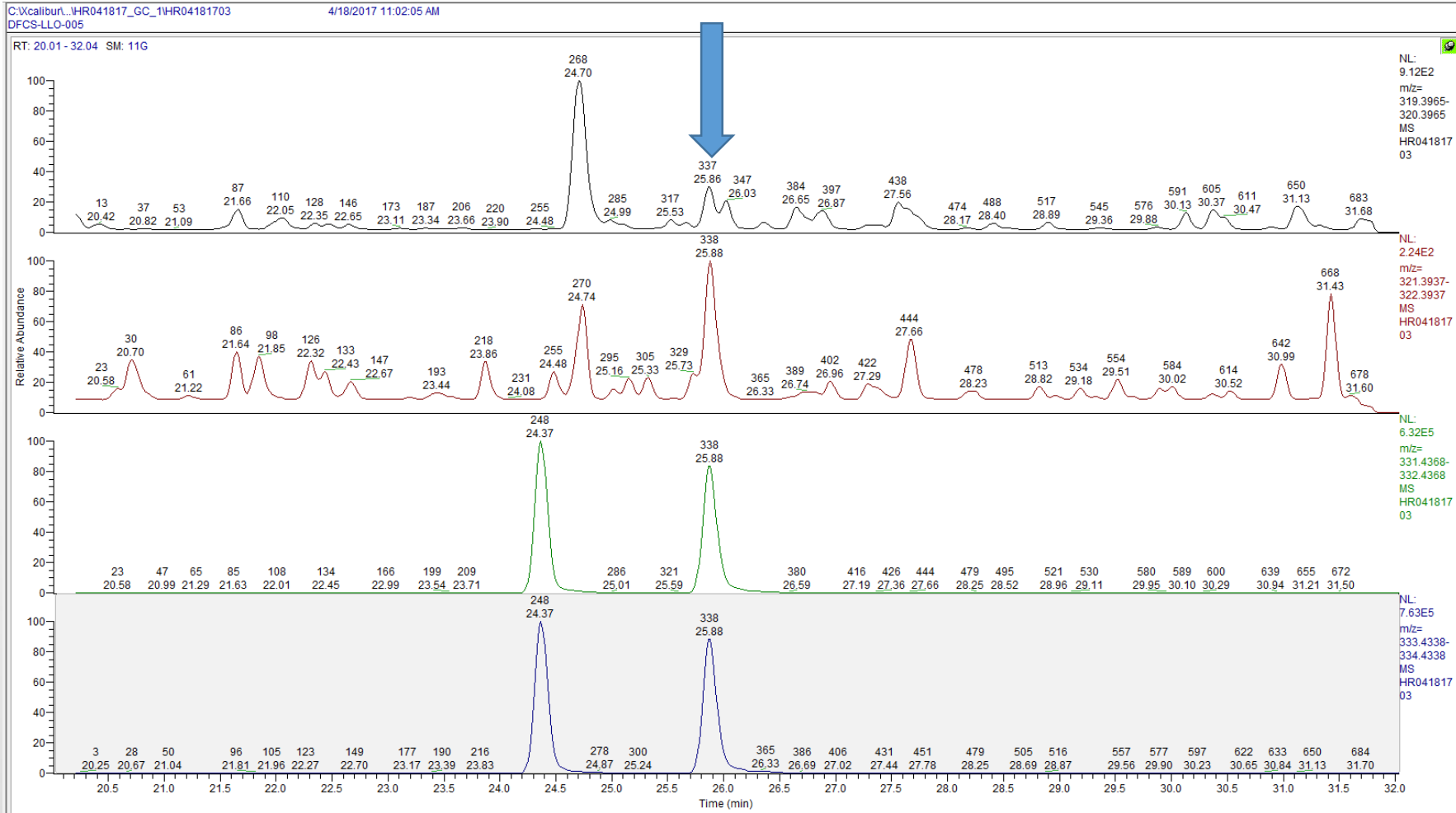


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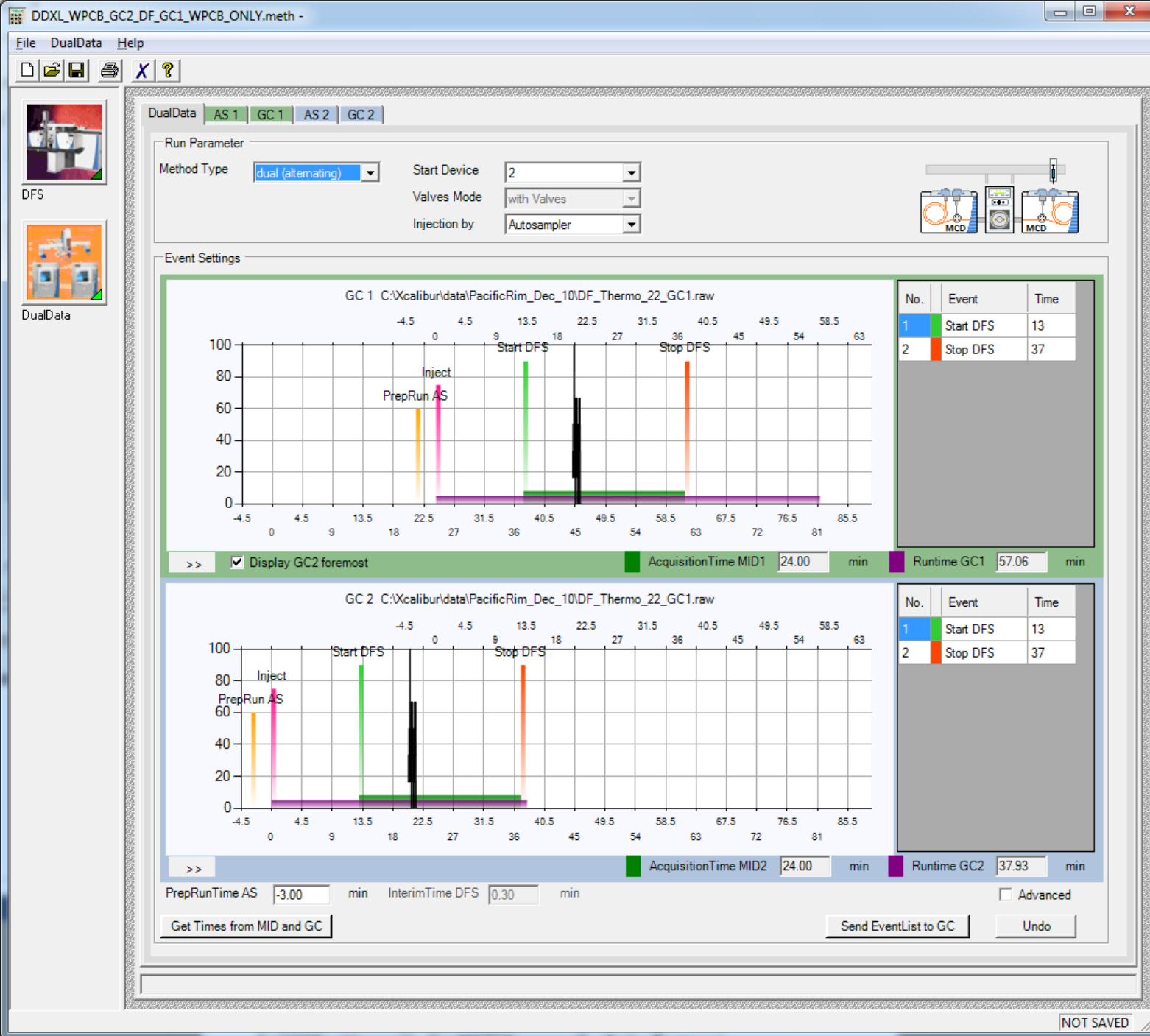
TCDD - CS-Lo 0.1 pg injected



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

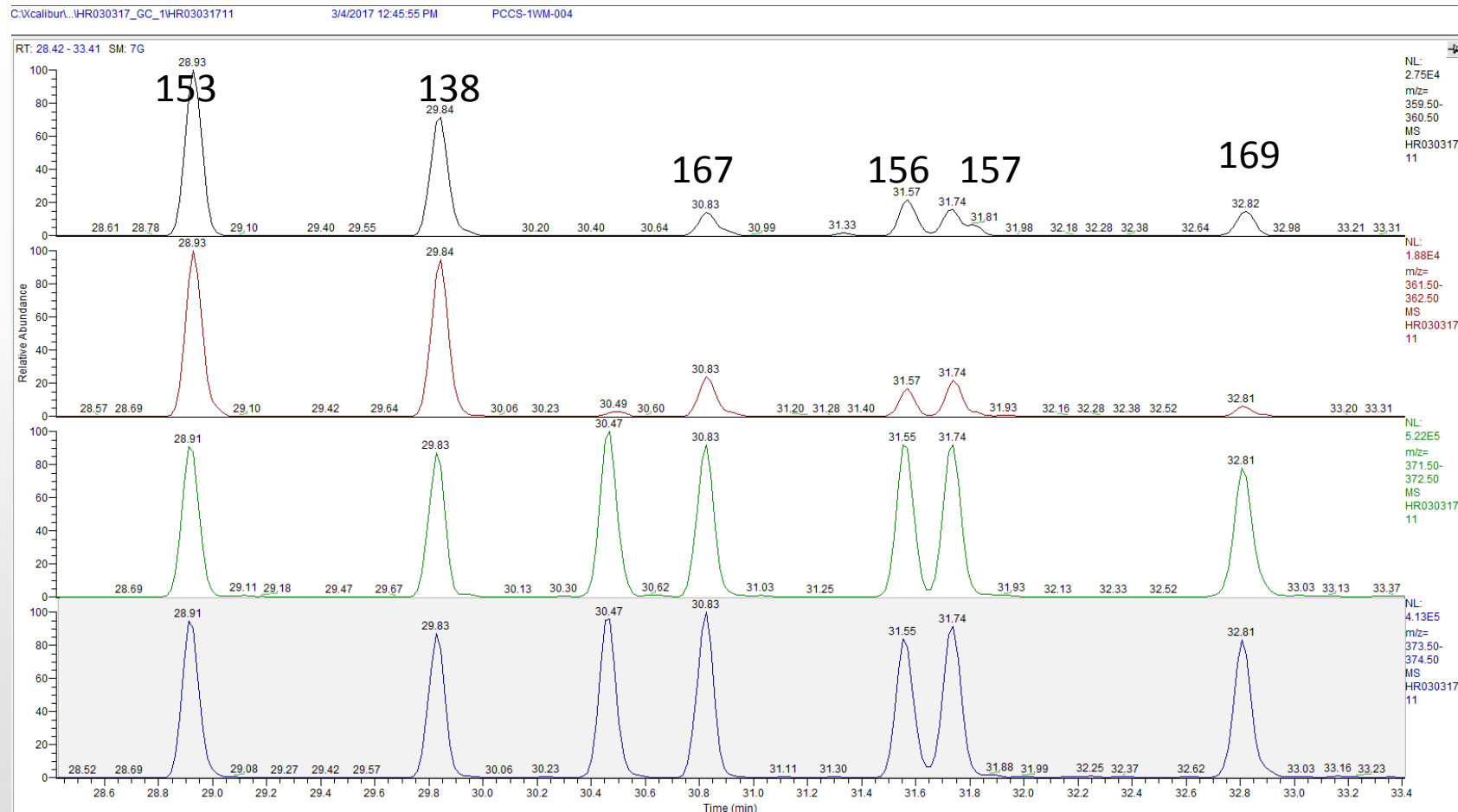
30 inj/day

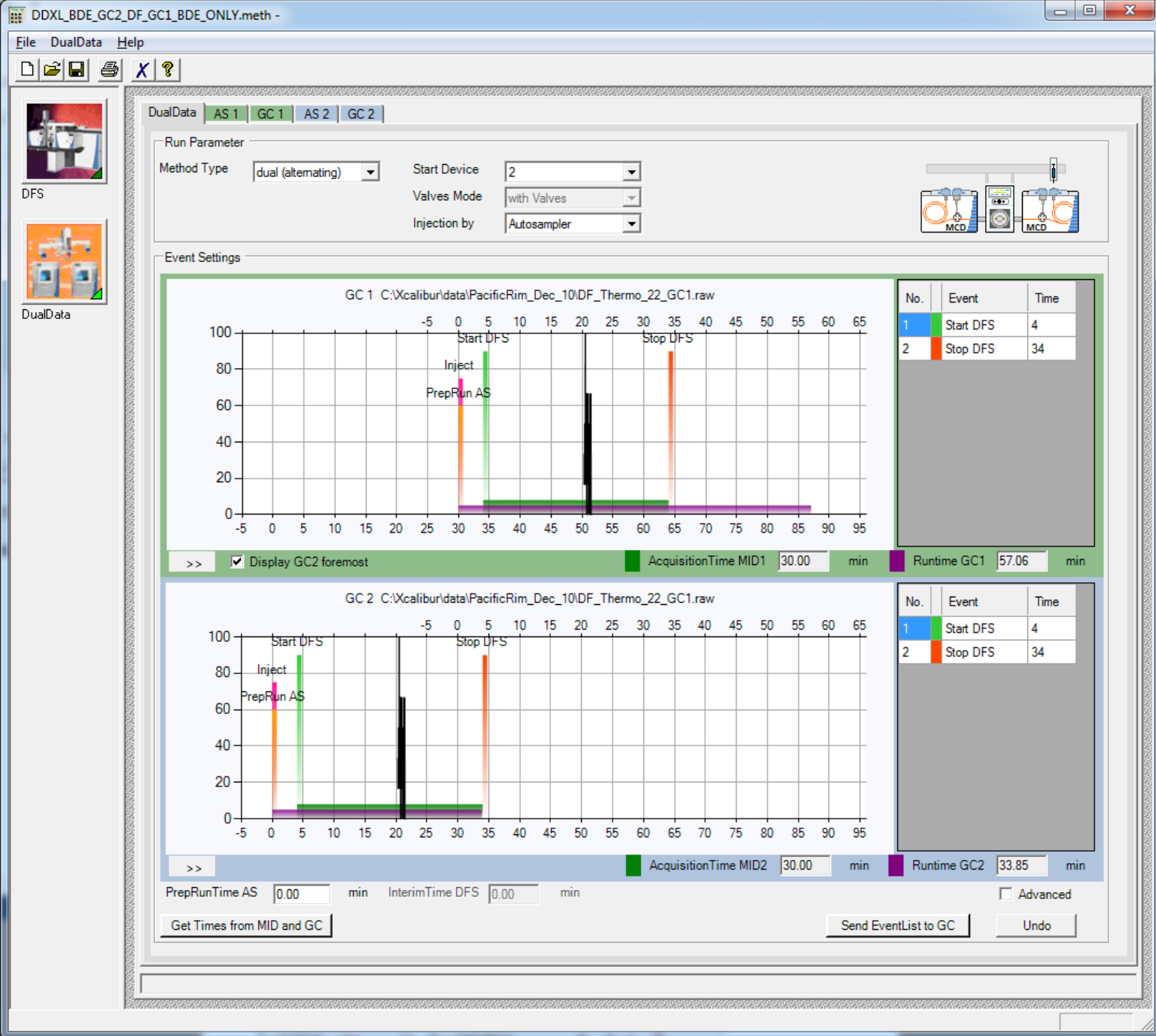
43% more analyses



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HxCB @ 0.1/0.5 pg injected





Dual BDE

Runtime DFS – 41 minutes (35 inj/day)

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

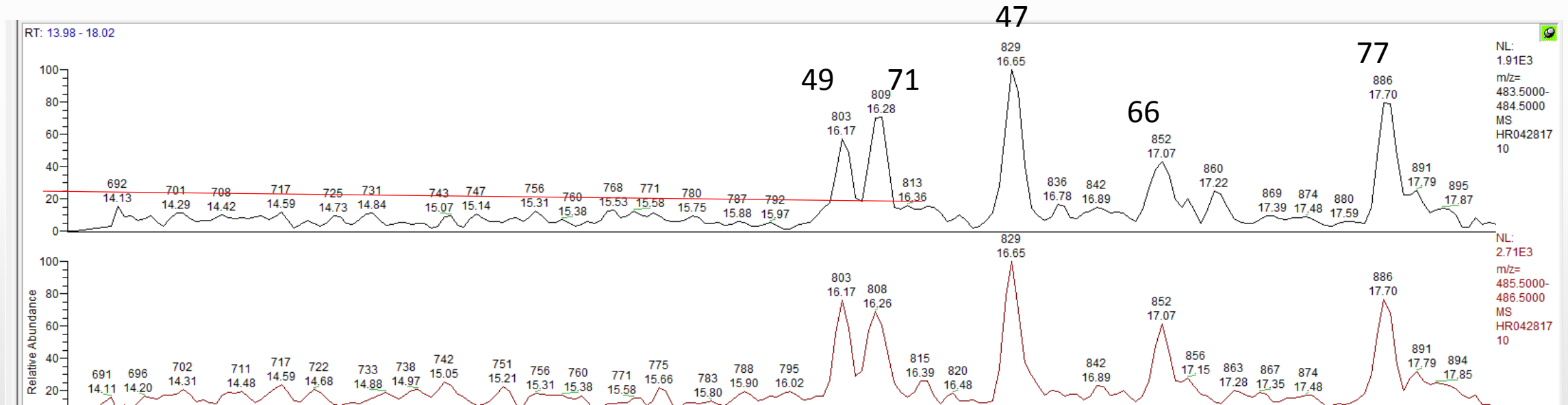
47 inj/day

34% more runs!



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TeBDE @ 0.5 pg injected

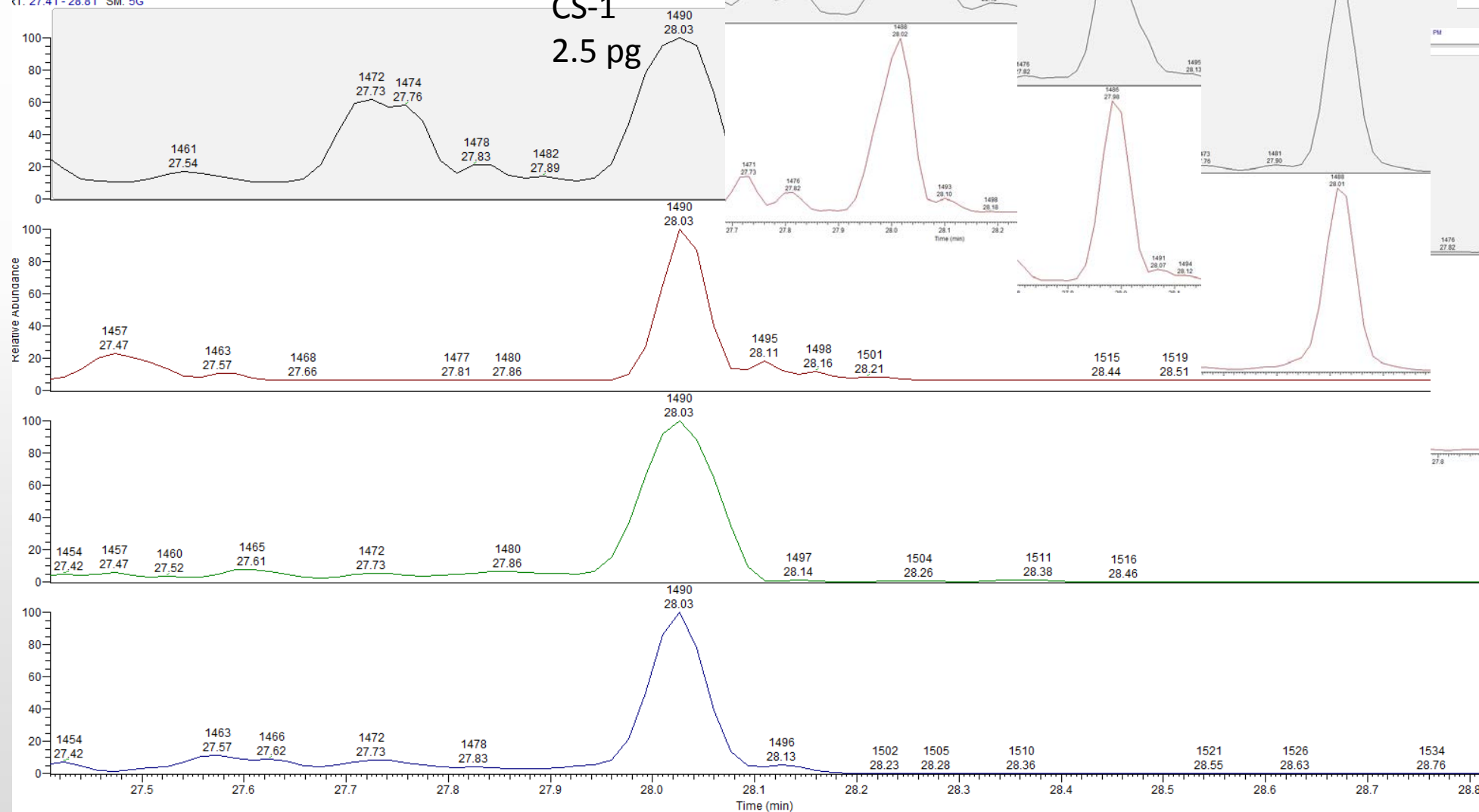


DecaDBE

4/29/2017 3:25:02 PM

RT: 27.41 - 28.81 SM: 5G

CS-1
2.5 pg



NL: 4.0000

PM

MS

HR042817

05

MS

HR042817

05

MS

HR042817

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HR042817

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HR042817

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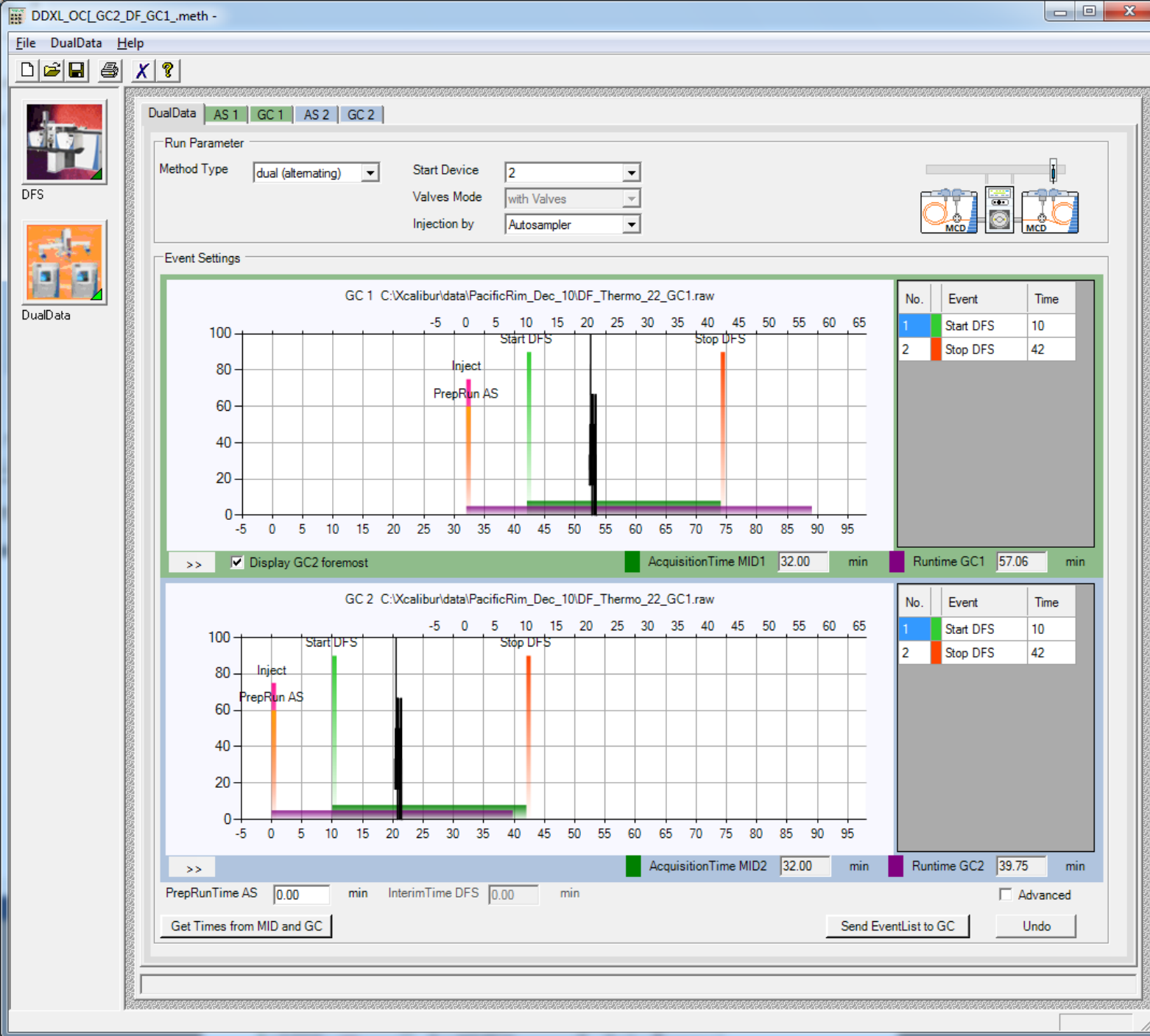
MS

HR042817

05



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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

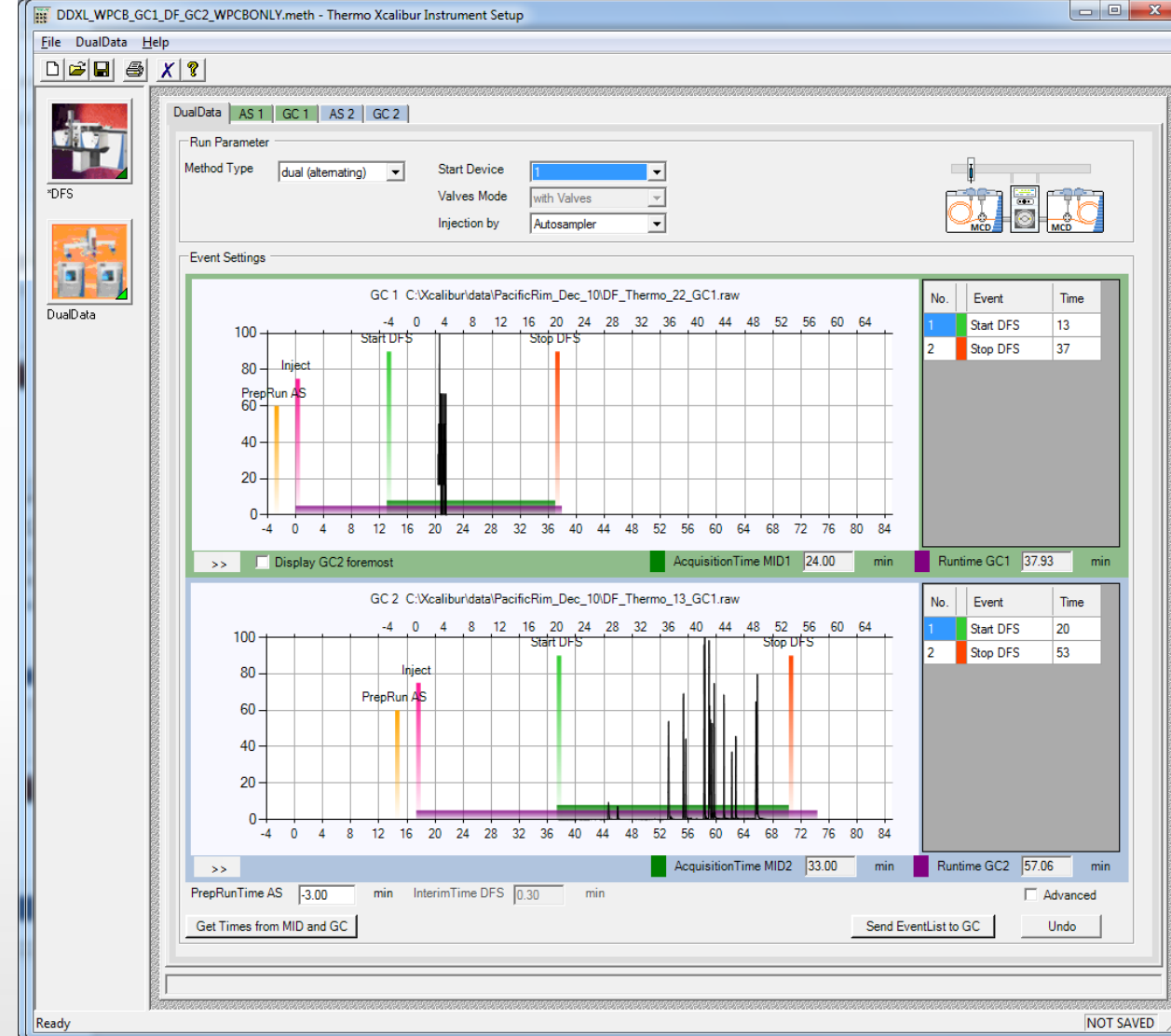
PCDD/F & dIPCB

PCDD/F Runtime DFS – 62 minutes

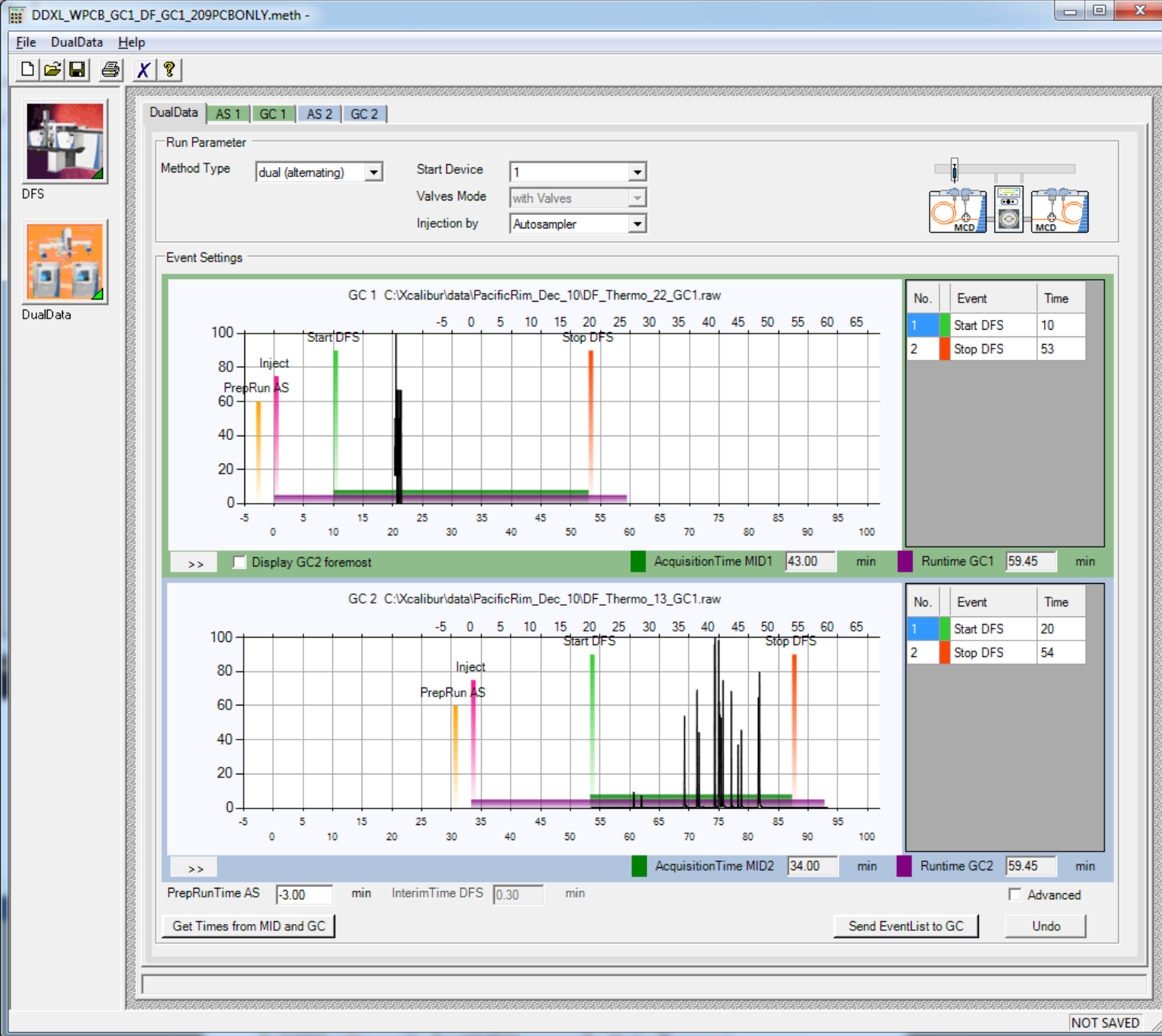
PCB Runtime DFS – 48 minutes

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

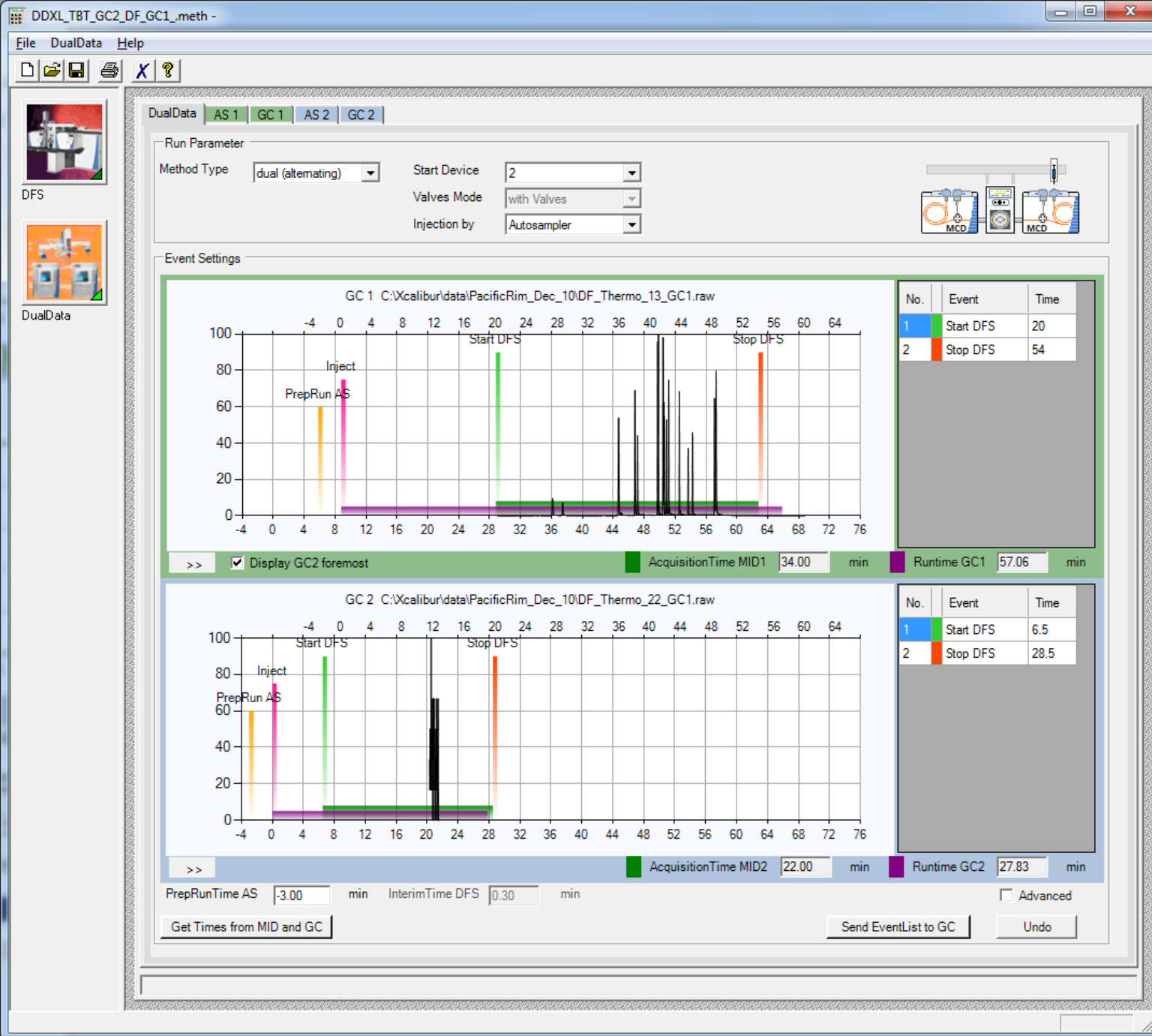
PCDD/F Runtime DFS – 62 minutes

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

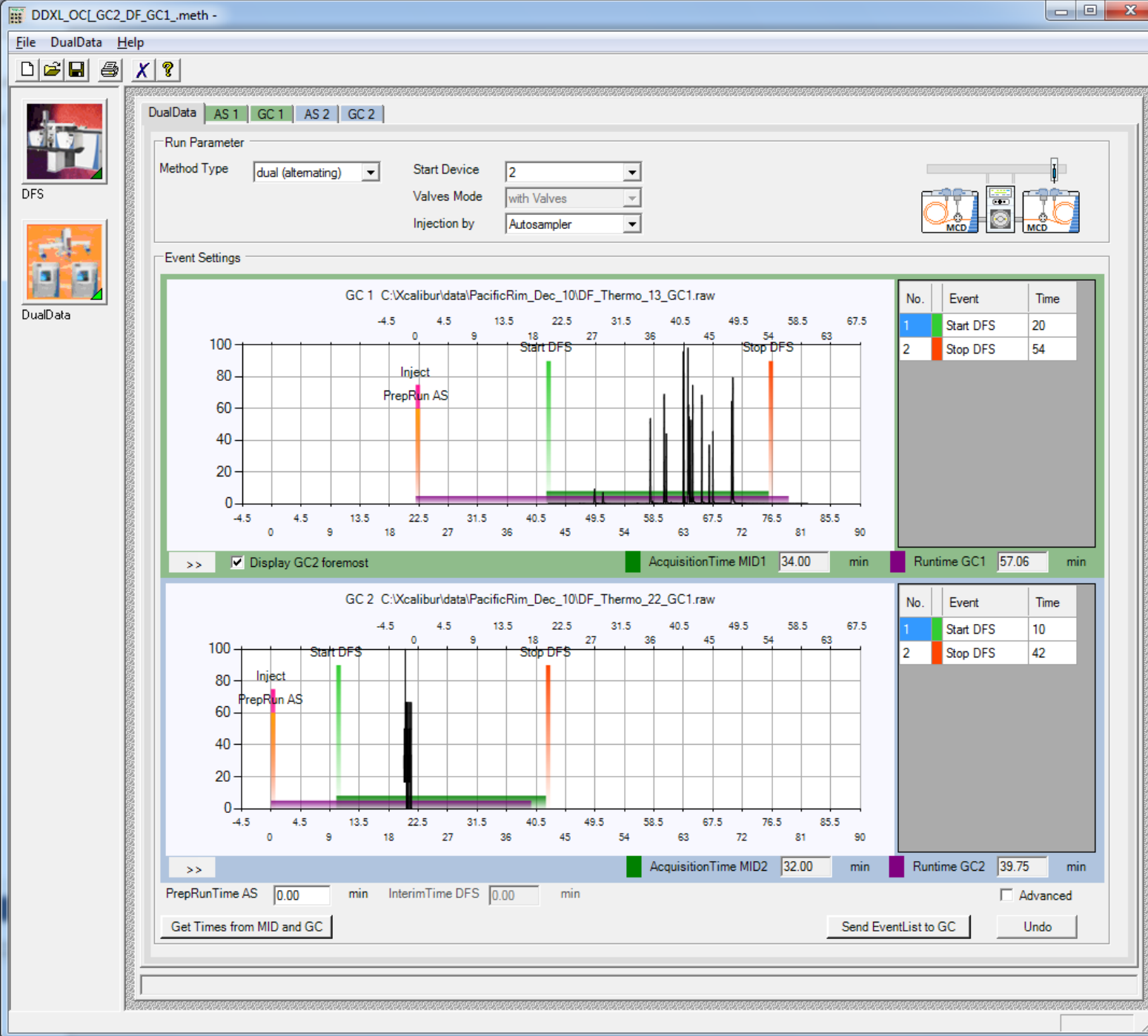
TBT Runtime DFS – 30 minutes

Runtime DualData XL – 56 minutes*

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



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PCDD/F & OCP

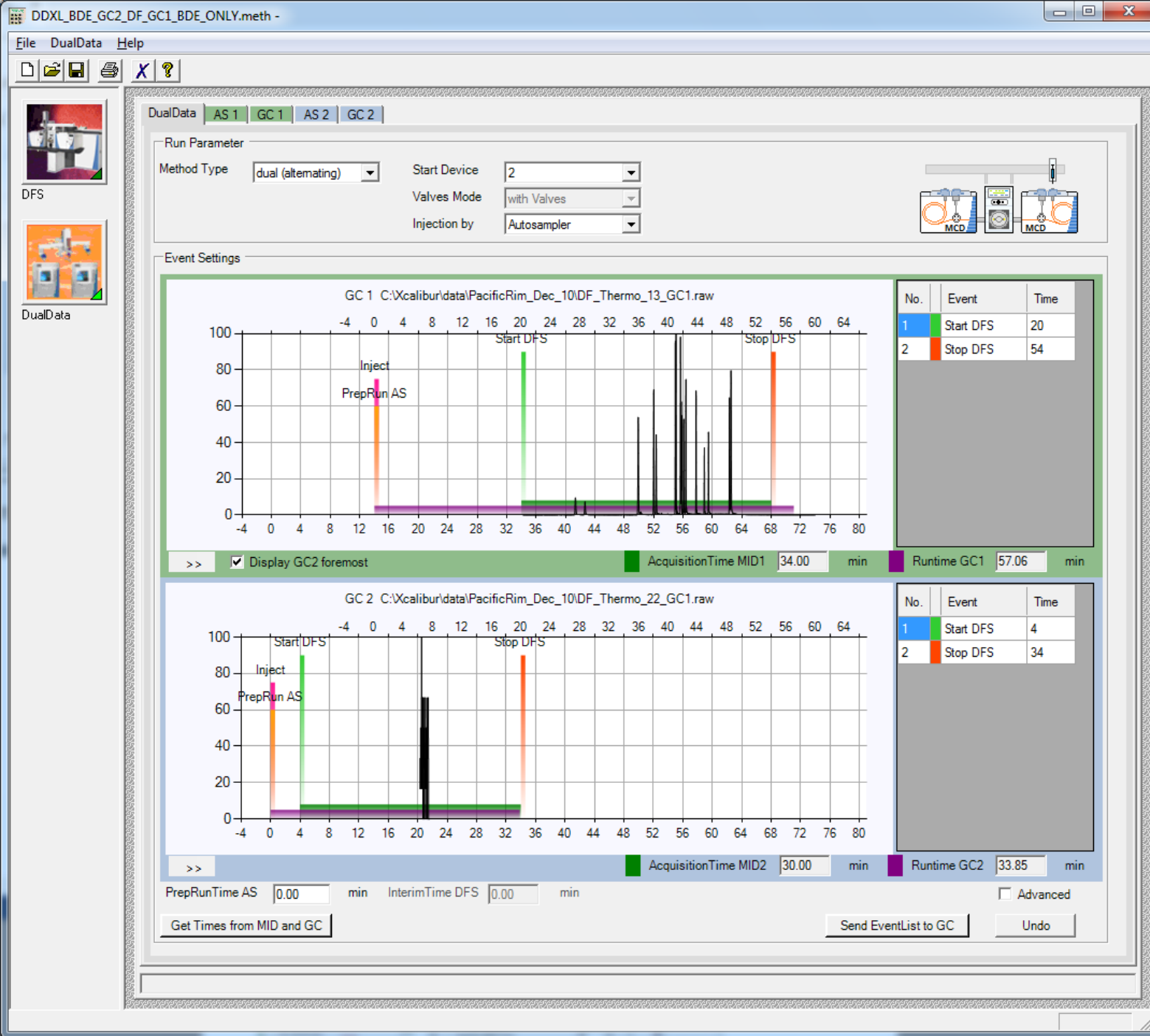
PCDD/F Runtime DFS – 62 minutes

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

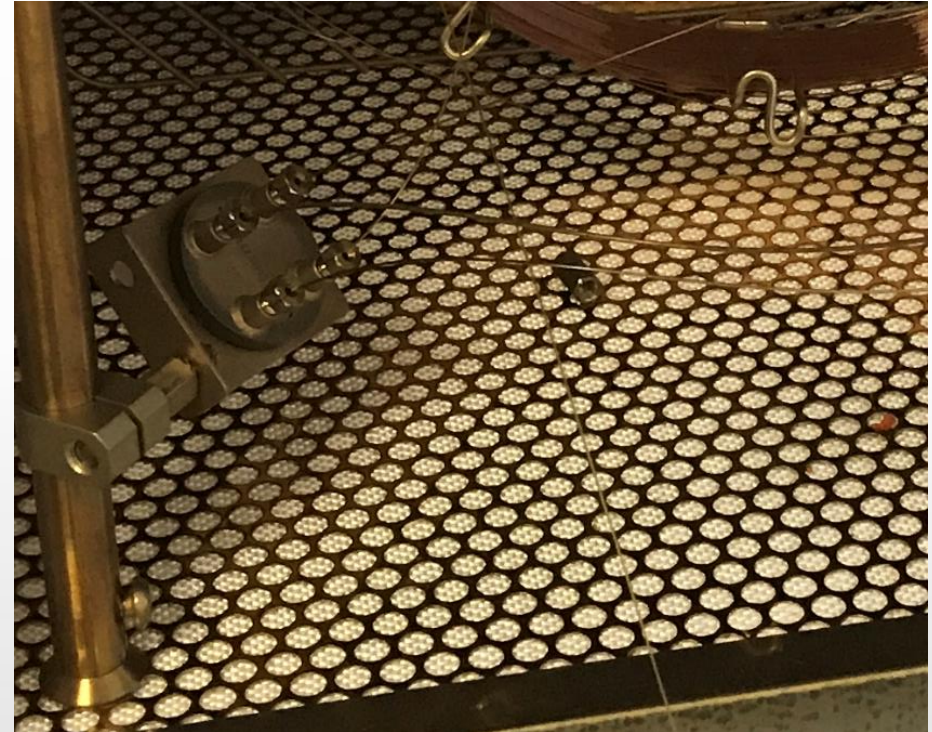
In our lab we use different tuning compound for PBDE v dioxin, so would never run together. This is just an example of what could be done.



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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



DI**XIN 2017**

Vancouver, Canada

August 20 -25, 2017

www.dioxin2017.org



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Thank you from Pacific Rim Labs.



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