GC Triple Quadrupole use in Challenging Matrices for Detection of Compounds in EPA Methods 8270, 8081 and 8082

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GCMS Applications
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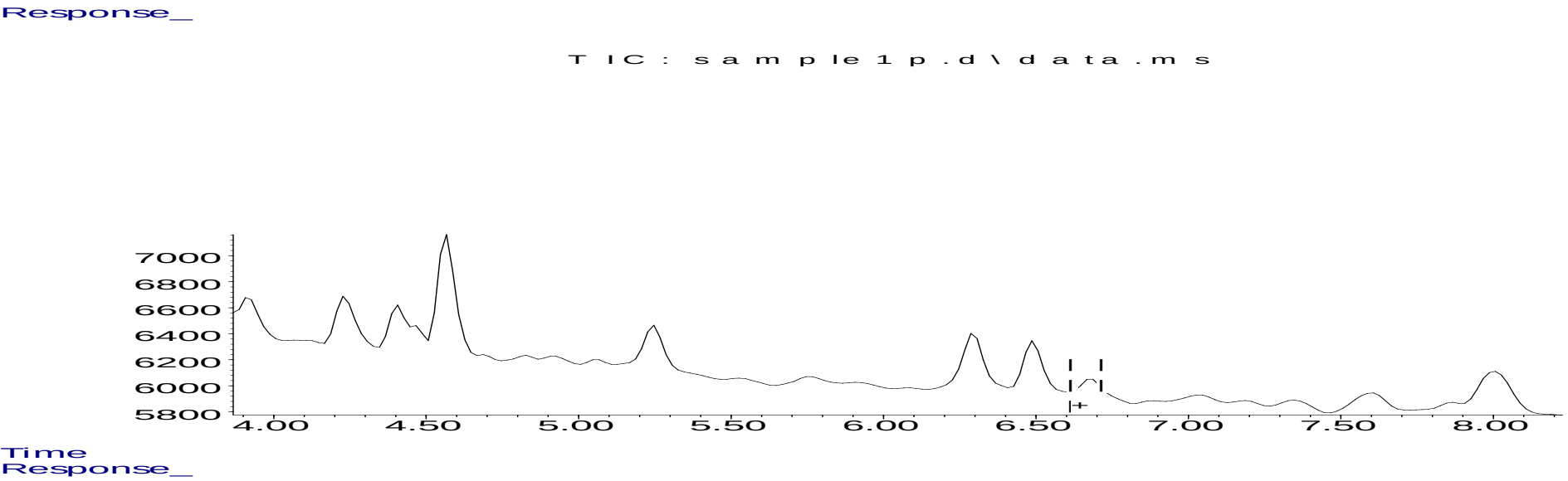
Project Scope
Convert Methods to GC-QQQ

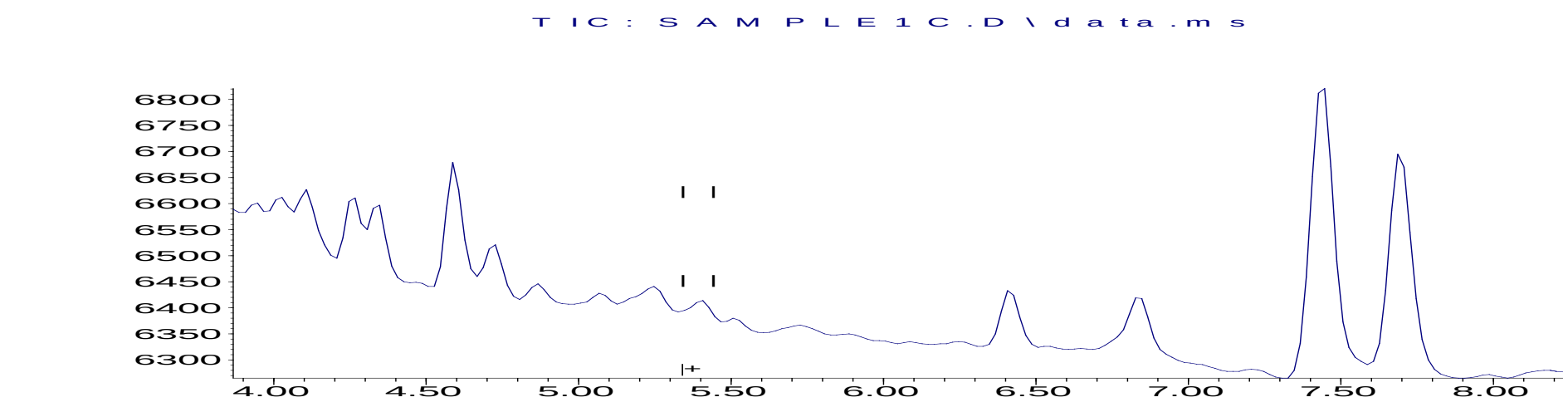
- **Chlorinated Pesticides – Method 8081**
  - **Including Toxaphene**
- **PCB Arochlors – Method 8082**
- **Organo-Phosphorus Pesticides – Method 8141**
- **Selected Semivolatiles – Method 8270**

Why are we doing this?

- **Eliminate matrix interferences**
- **Achieve lower levels of detection**
- **Simplify data review**
- **Faster analysis times**

Typical Dual Column ECD Sample – Gamma BHC Method 8081 Chlorinated Pesticides





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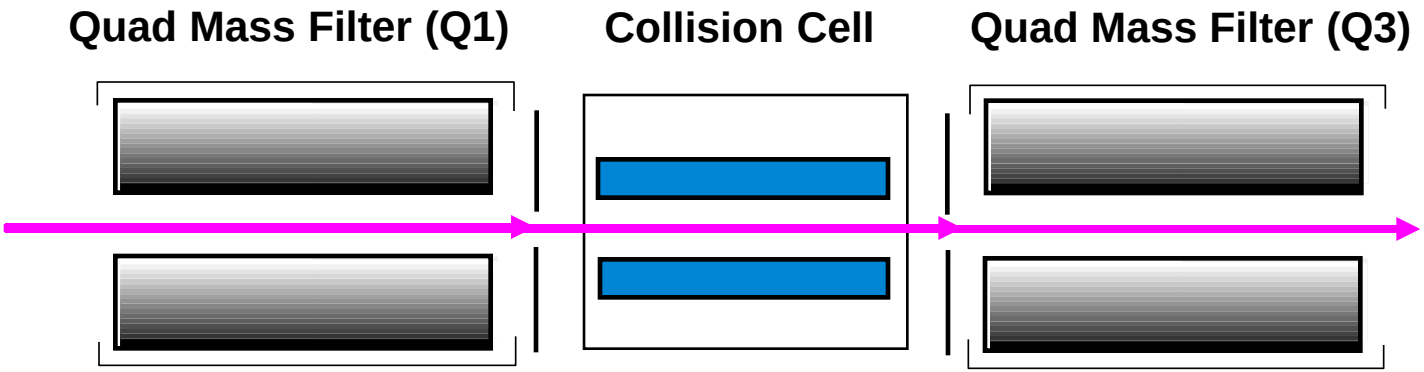
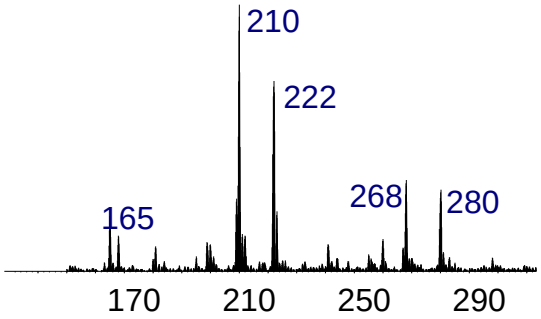
Multiple Reaction Monitoring (MRM)

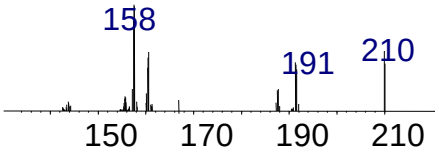


Spectrum with background ions (from EI)

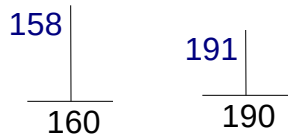


Q1 lets **only** target ion 210 pass through

Collision cell breaks ion 210 apart



Q3 monitors **only** characteristic fragments 158 and 191 from ion 210 for quant and qual.



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What is a Transition?

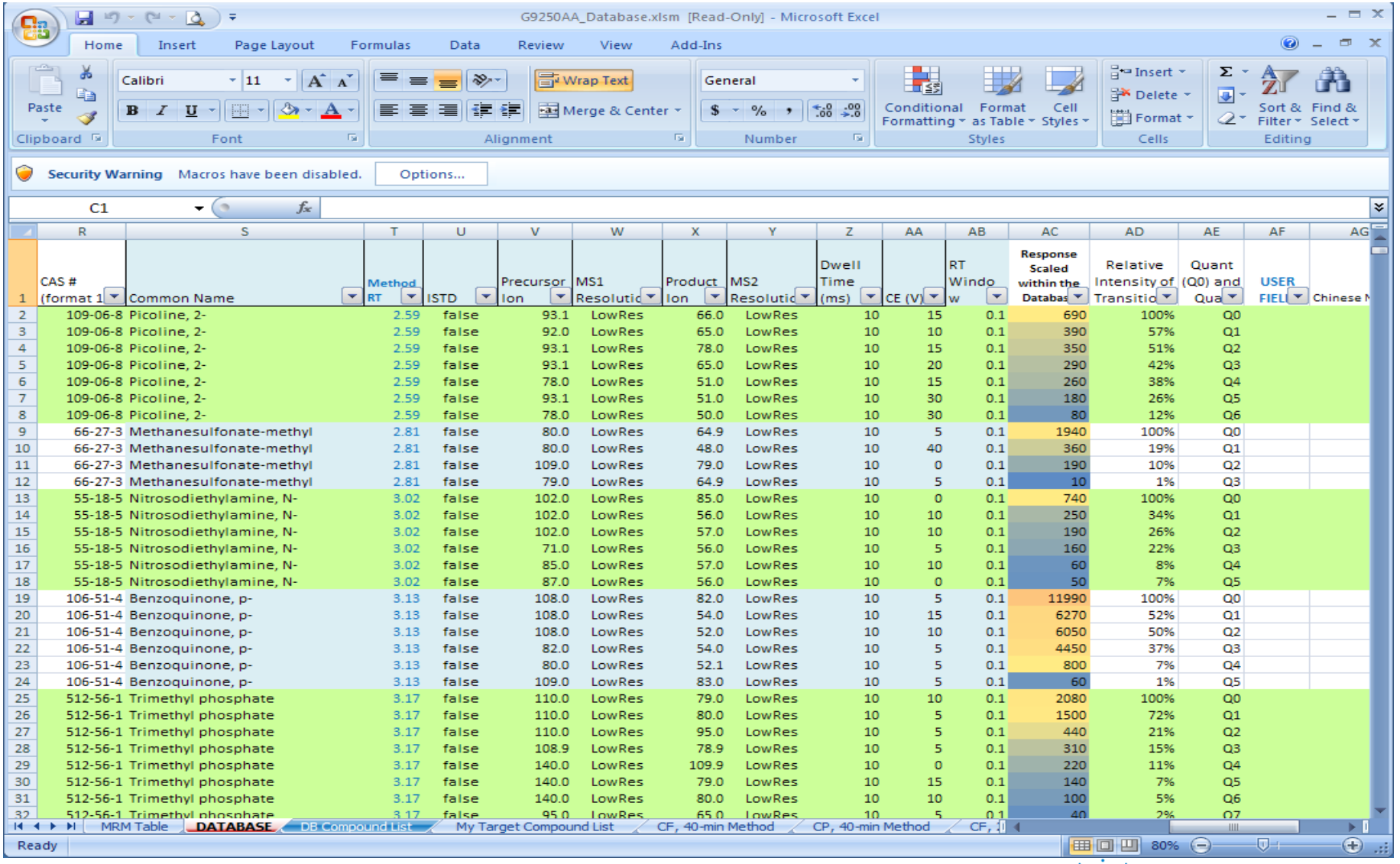
- **Transitions consist of a Precursor ion – Collision Energy – Product Ion**

- **In the previous example transitions would be:**
  - **210 → 158**
  - **210 → 191**

- **Typically two transitions are used for each analyte**
- **Transitions often abbreviated to MRM**
  - **Multiple Reaction Monitoring**

- **Where do Transitions come from?**
  - **Develop your own**
  - **Transition Database**

G9250AA Transition Database
1000 Compounds – up to Eight Transitions each



	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
1	CAS # (format 1	Common Name	Method RT	ISTD	Precursor Ion	MS1 Resolutio	Product Ion	MS2 Resolutio	Dwell Time (ms)	CE (V)	RT Windo w	Response Scaled within the Databas	Relative Intensity of Transitio	Quant (Q0) and Qua	USER FIEL	Chinese
2	109-06-8	Picoline, 2-	2.59	false	93.1	LowRes	66.0	LowRes	10	15	0.1	690	100%	Q0		
3	109-06-8	Picoline, 2-	2.59	false	92.0	LowRes	65.0	LowRes	10	10	0.1	390	57%	Q1		
4	109-06-8	Picoline, 2-	2.59	false	93.1	LowRes	78.0	LowRes	10	15	0.1	350	51%	Q2		
5	109-06-8	Picoline, 2-	2.59	false	93.1	LowRes	65.0	LowRes	10	20	0.1	290	42%	Q3		
6	109-06-8	Picoline, 2-	2.59	false	78.0	LowRes	51.0	LowRes	10	15	0.1	260	38%	Q4		
7	109-06-8	Picoline, 2-	2.59	false	93.1	LowRes	51.0	LowRes	10	30	0.1	180	26%	Q5		
8	109-06-8	Picoline, 2-	2.59	false	78.0	LowRes	50.0	LowRes	10	30	0.1	80	12%	Q6		
9	66-27-3	Methanesulfonate-methyl	2.81	false	80.0	LowRes	64.9	LowRes	10	5	0.1	1940	100%	Q0		
10	66-27-3	Methanesulfonate-methyl	2.81	false	80.0	LowRes	48.0	LowRes	10	40	0.1	360	19%	Q1		
11	66-27-3	Methanesulfonate-methyl	2.81	false	109.0	LowRes	79.0	LowRes	10	0	0.1	190	10%	Q2		
12	66-27-3	Methanesulfonate-methyl	2.81	false	79.0	LowRes	64.9	LowRes	10	5	0.1	10	1%	Q3		
13	55-18-5	Nitrosodiethylamine, N-	3.02	false	102.0	LowRes	85.0	LowRes	10	0	0.1	740	100%	Q0		
14	55-18-5	Nitrosodiethylamine, N-	3.02	false	102.0	LowRes	56.0	LowRes	10	10	0.1	250	34%	Q1		
15	55-18-5	Nitrosodiethylamine, N-	3.02	false	102.0	LowRes	57.0	LowRes	10	10	0.1	190	26%	Q2		
16	55-18-5	Nitrosodiethylamine, N-	3.02	false	71.0	LowRes	56.0	LowRes	10	5	0.1	160	22%	Q3		
17	55-18-5	Nitrosodiethylamine, N-	3.02	false	85.0	LowRes	57.0	LowRes	10	10	0.1	60	8%	Q4		
18	55-18-5	Nitrosodiethylamine, N-	3.02	false	87.0	LowRes	56.0	LowRes	10	0	0.1	50	7%	Q5		
19	106-51-4	Benzoquinone, p-	3.13	false	108.0	LowRes	82.0	LowRes	10	5	0.1	11990	100%	Q0		
20	106-51-4	Benzoquinone, p-	3.13	false	108.0	LowRes	54.0	LowRes	10	15	0.1	6270	52%	Q1		
21	106-51-4	Benzoquinone, p-	3.13	false	108.0	LowRes	52.0	LowRes	10	10	0.1	6050	50%	Q2		
22	106-51-4	Benzoquinone, p-	3.13	false	82.0	LowRes	54.0	LowRes	10	5	0.1	4450	37%	Q3		
23	106-51-4	Benzoquinone, p-	3.13	false	80.0	LowRes	52.1	LowRes	10	5	0.1	800	7%	Q4		
24	106-51-4	Benzoquinone, p-	3.13	false	109.0	LowRes	83.0	LowRes	10	5	0.1	60	1%	Q5		
25	512-56-1	Trimethyl phosphate	3.17	false	110.0	LowRes	79.0	LowRes	10	10	0.1	2080	100%	Q0		
26	512-56-1	Trimethyl phosphate	3.17	false	110.0	LowRes	80.0	LowRes	10	5	0.1	1500	72%	Q1		
27	512-56-1	Trimethyl phosphate	3.17	false	110.0	LowRes	95.0	LowRes	10	5	0.1	440	21%	Q2		
28	512-56-1	Trimethyl phosphate	3.17	false	108.9	LowRes	78.9	LowRes	10	5	0.1	310	15%	Q3		
29	512-56-1	Trimethyl phosphate	3.17	false	140.0	LowRes	109.9	LowRes	10	0	0.1	220	11%	Q4		
30	512-56-1	Trimethyl phosphate	3.17	false	140.0	LowRes	79.0	LowRes	10	15	0.1	140	7%	Q5		
31	512-56-1	Trimethyl phosphate	3.17	false	140.0	LowRes	80.0	LowRes	10	10	0.1	100	5%	Q6		
32	512-56-1	Trimethyl phosphate	3.17	false	95.0	LowRes	65.0	LowRes	10	5	0.1	40	2%	Q7		

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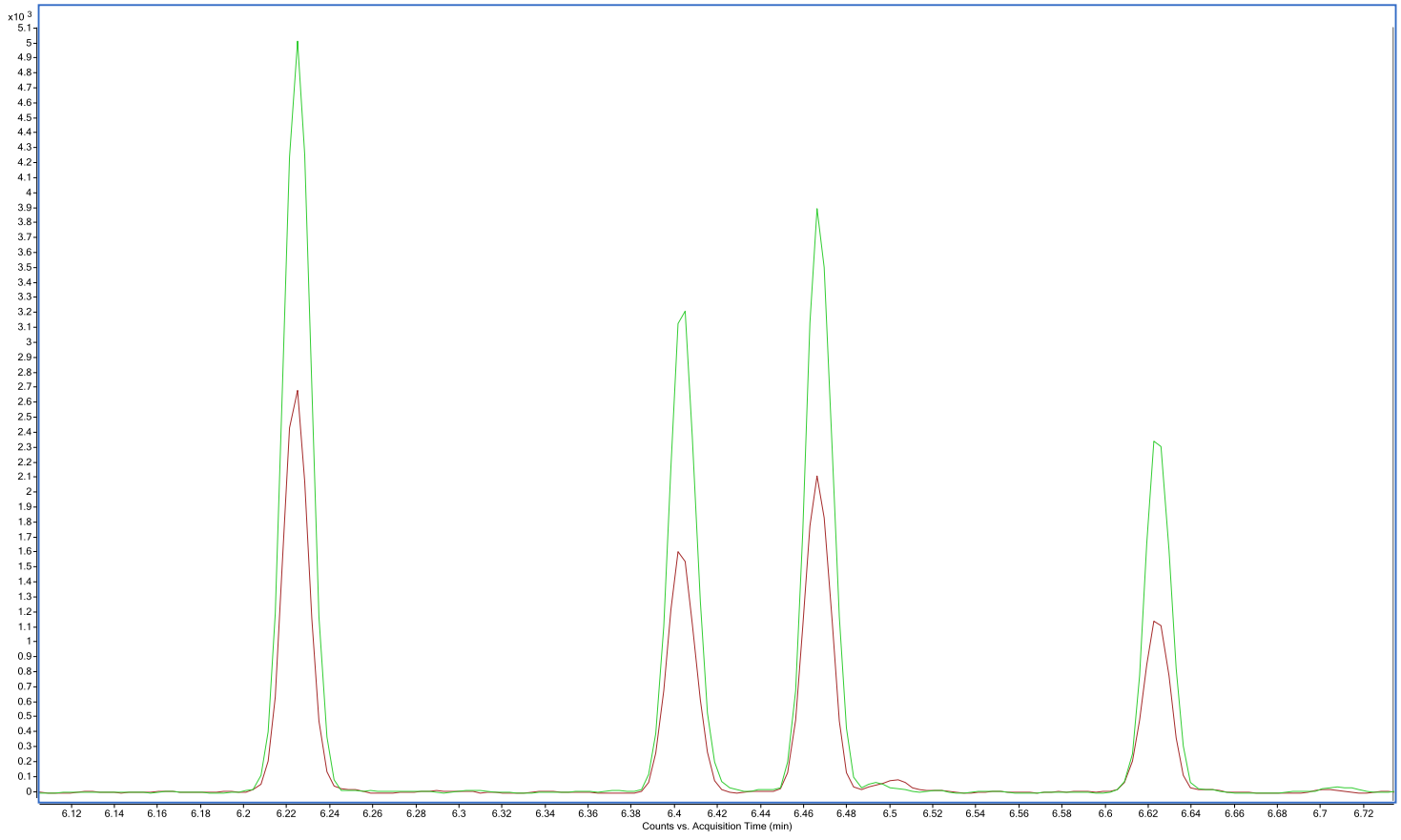
Method 8081

- **Enough sensitivity to match ECD levels?**
- **Linearity?**
- **Meet MDL requirements**
- **Eliminate interferences**

Enough Sensitivity?
BHCs at 1 pg on-column
181 → 109 181 → 145



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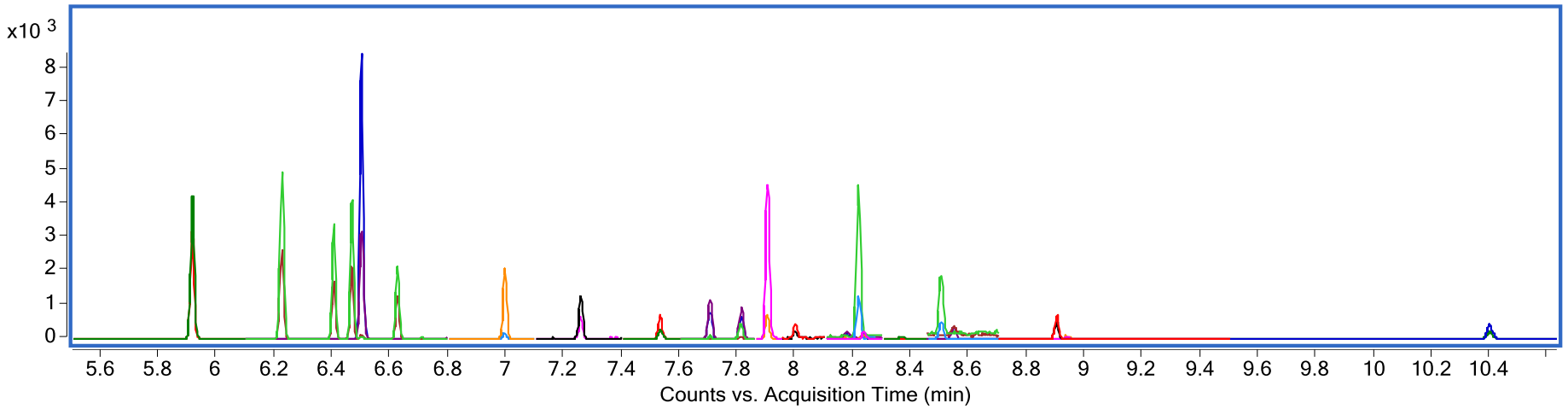
8081 STD 1.0 pg/ul



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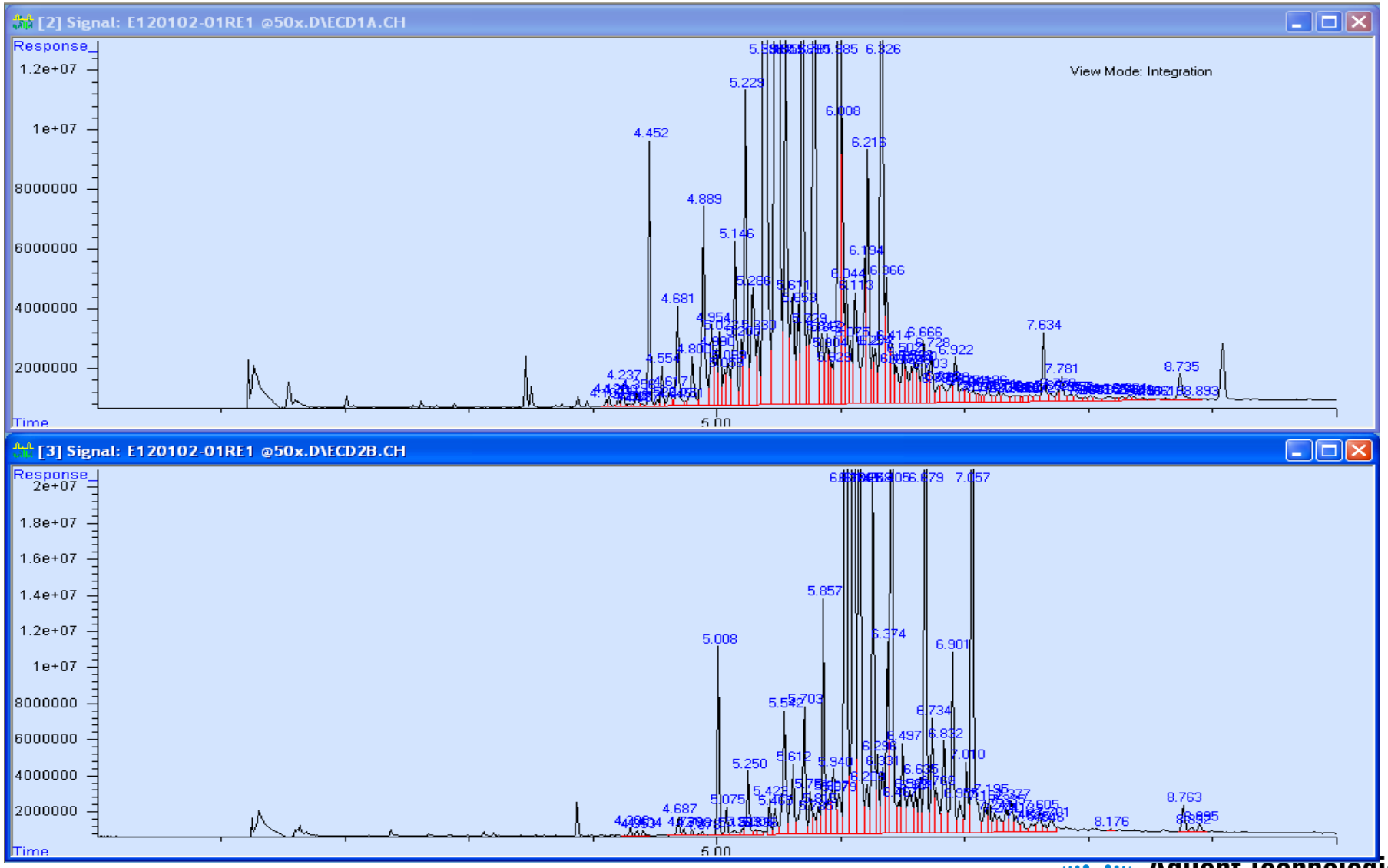
Method 8081 IDL

Compound								ave	std	mdl	% rsd
TCMX	1.40	1.49	1.40	1.45	1.44	1.42	1.46	1.44	0.03	0.11	2.41
BHC a	2.01	2.02	1.98	2.00	2.02	1.94	2.07	2.00	0.04	0.12	1.92
BHC-b	2.40	2.42	2.39	2.41	2.39	2.43	2.41	2.41	0.01	0.05	0.60
BHC-g	2.45	2.50	2.40	2.48	2.44	2.45	2.48	2.46	0.03	0.10	1.32
BHC-d	3.17	3.18	3.09	3.13	3.14	3.13	3.11	3.14	0.03	0.10	1.02
Heptachlor	2.06	2.11	2.01	1.99	2.05	1.98	2.06	2.04	0.05	0.15	2.30
Aldrin	2.54	2.47	2.44	2.47	2.43	2.48	2.51	2.48	0.04	0.12	1.60
Heptachlor Epoxide	2.97	2.84	2.84	2.84	2.91	2.78	2.83	2.86	0.06	0.19	2.13
Chlordane-trans	3.58	3.57	3.49	3.44	3.48	3.49	3.51	3.51	0.05	0.16	1.44
Endosulfan I	3.48	3.47	3.35	3.45	3.42	3.45	3.53	3.45	0.06	0.18	1.67
Chlordane-cis	4.11	4.13	4.03	4.07	4.01	4.00	4.03	4.05	0.05	0.16	1.29
DDE	4.48	4.47	4.42	4.43	4.45	4.43	4.44	4.45	0.02	0.06	0.46
Dieldrin	3.13	3.03	2.88	2.96	3.08	3.07	3.00	3.02	0.08	0.26	2.74
Endrin	1.84	2.40	1.59	1.67	2.07	1.74	1.37	1.81	0.34	1.07	18.75
DDD	4.40	4.37	4.29	4.31	4.31	4.28	4.31	4.32	0.04	0.14	1.00
Endosulfan II	4.76	4.66	4.51	4.46	4.55	4.75	4.67	4.62	0.12	0.37	2.56
Endrin Aldehyde	3.34	3.23	3.29	3.15	3.11	3.21	3.10	3.20	0.09	0.28	2.80
DDT	3.71	3.67	3.62	3.63	3.64	3.60	3.61	3.64	0.04	0.12	1.09
Endosulfan Sulfate	5.32	5.23	5.12	5.11	5.10	5.14	5.03	5.15	0.10	0.30	1.86
Methoxychlor	2.68	2.48	2.40	2.39	2.35	2.39	2.38	2.44	0.11	0.36	4.69
Endrin Ketone	3.92	3.65	4.03	3.85	3.82	3.80	3.80	3.84	0.12	0.37	3.06
DCB	3.92	3.72	3.68	3.66	3.58	3.57	3.62	3.68	0.12	0.38	3.25

Pesticide Production Facility #1 On ECD



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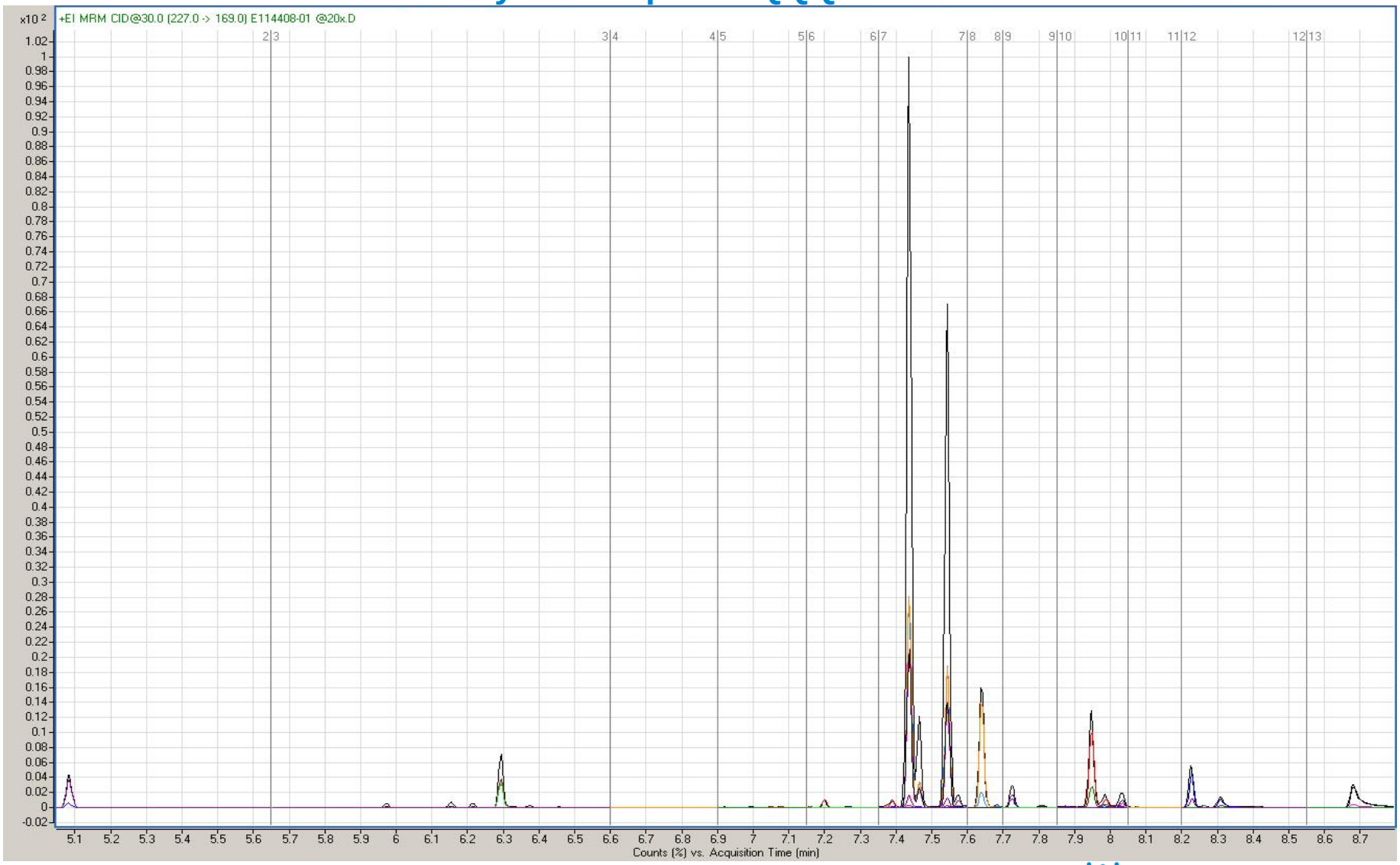
Pesticide Production Facility #1 Sample on QQQ



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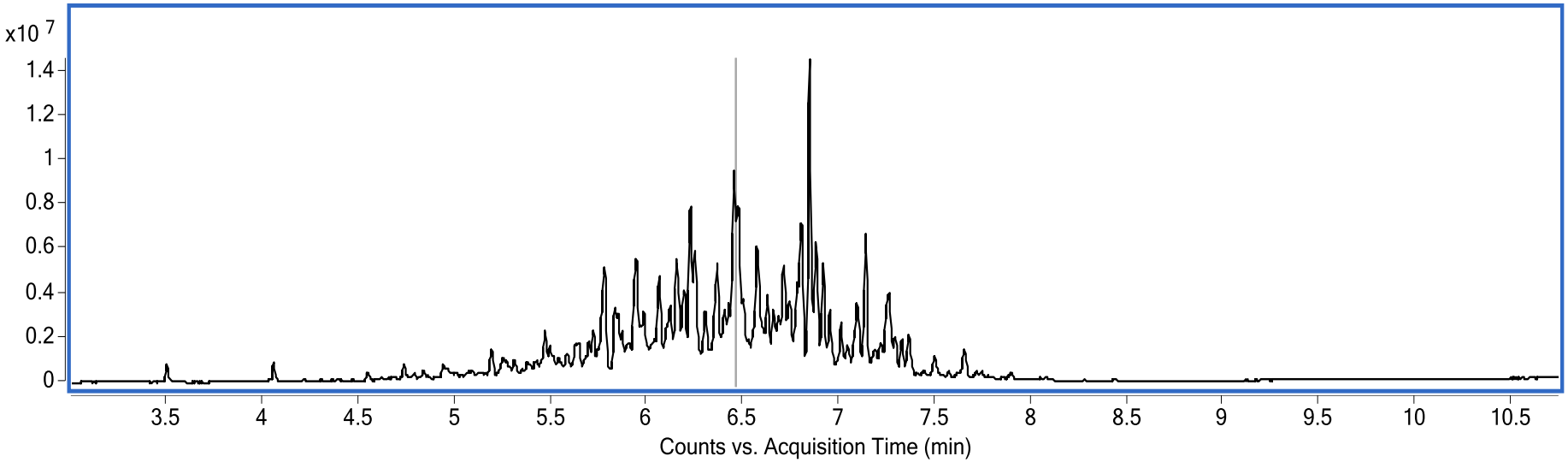
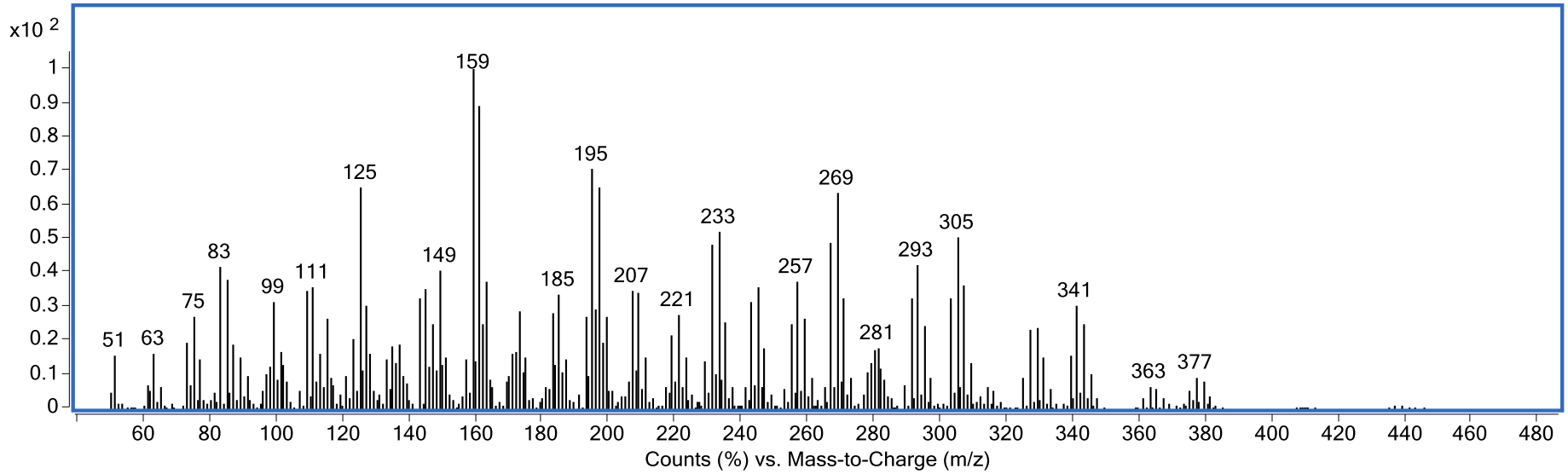
What about Multicomponent Analytes?

- **Method 8081:**
- **Toxaphene**
  - **Chlorinated Camphene (over 600 individual congeners)**
- **Chlordanes**
- **Method 8082:**
- **PCB Arochlors are mixtures of congeners (209 individual congeners)**
  - **Different isomers and different levels of chlorination**

Toxaphene Full Scan





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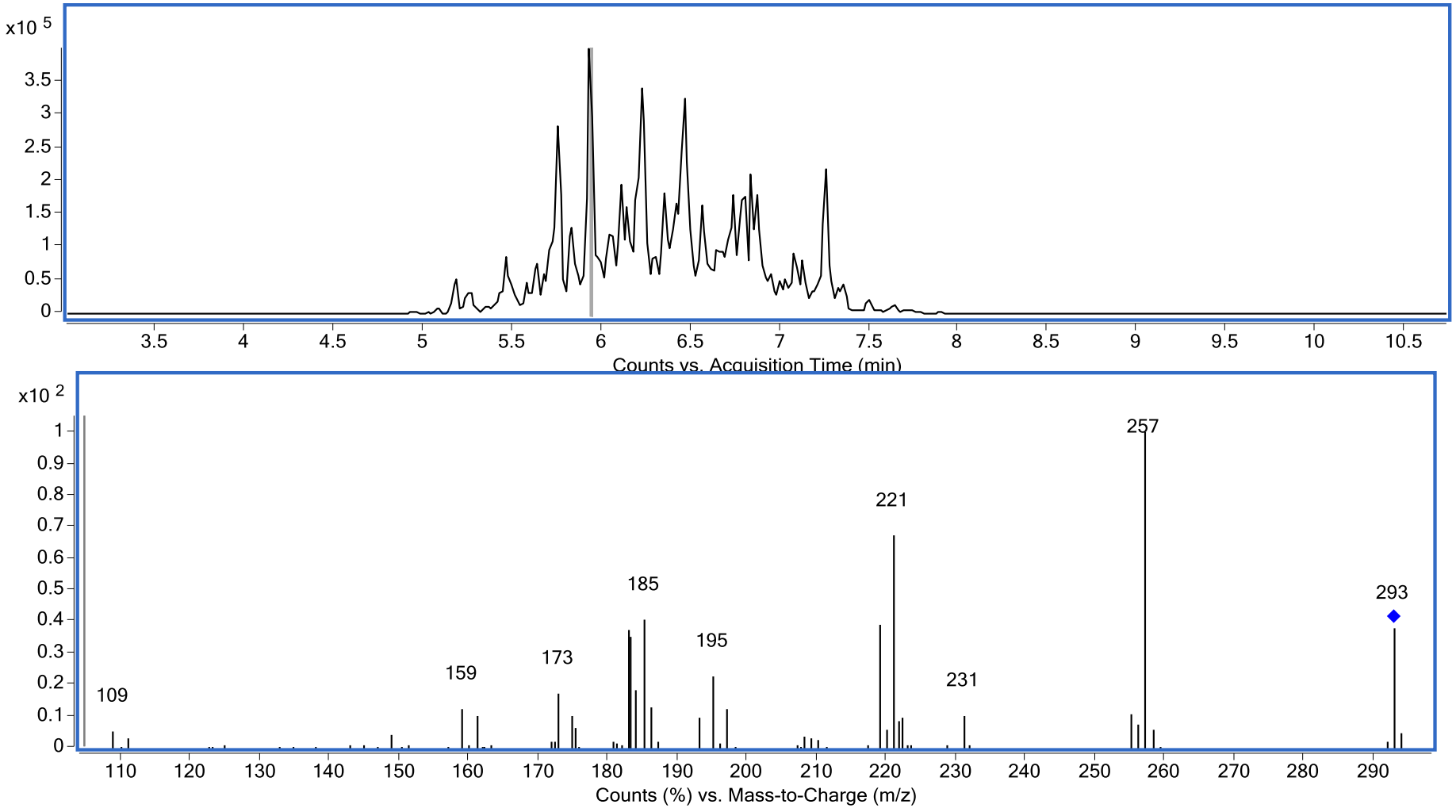
Toxaphene Product Ion Scan from 293 Precursor



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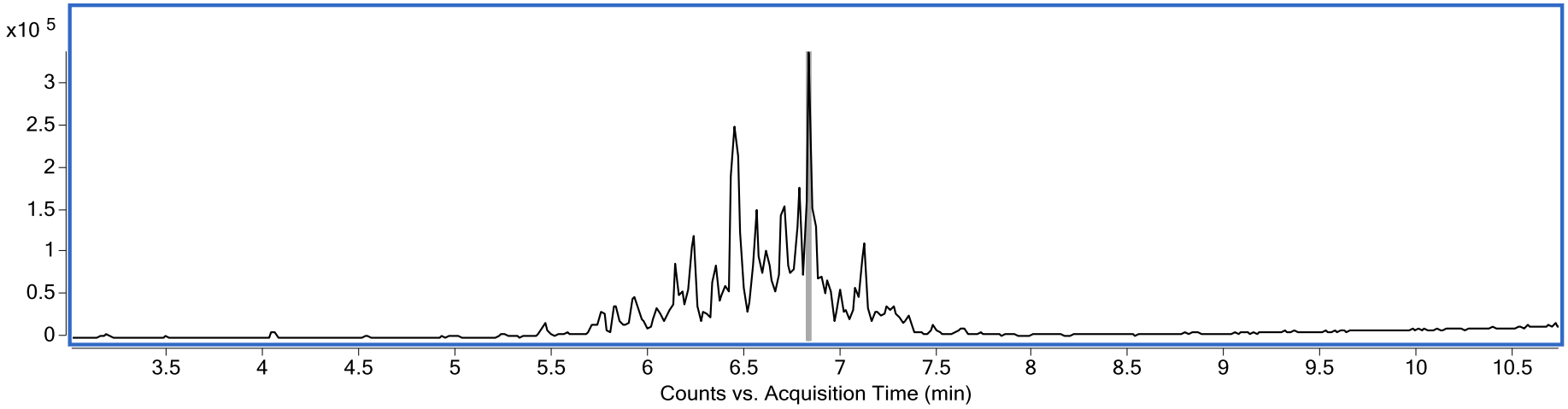
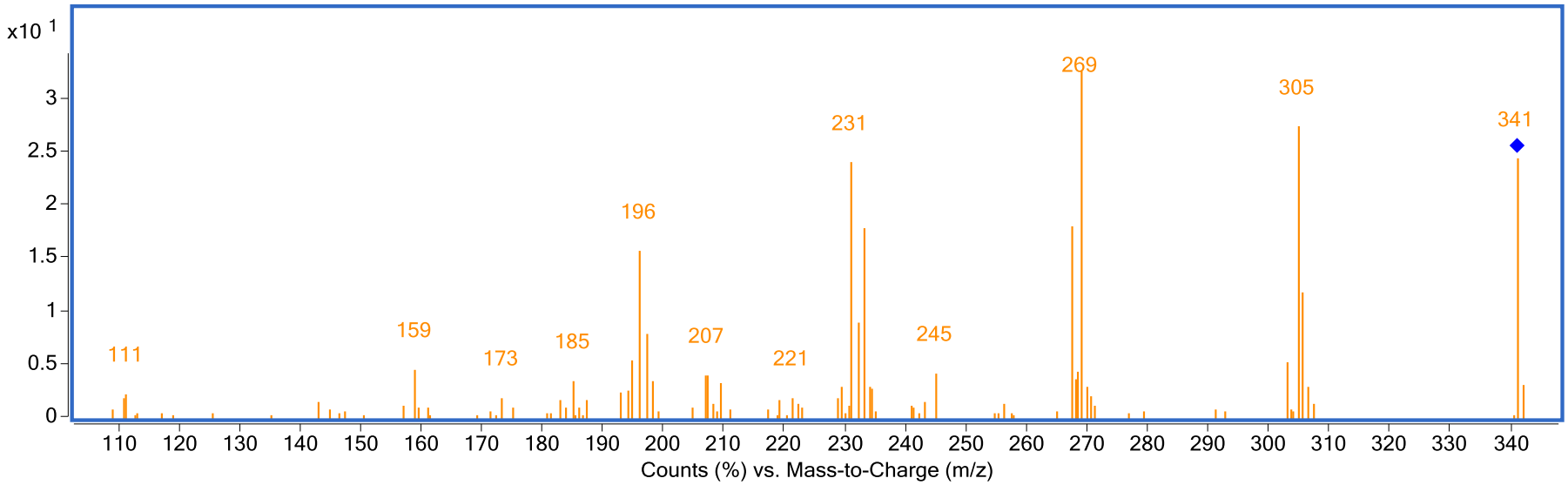
Toxaphene Product Ion Scan from 341 Precursor





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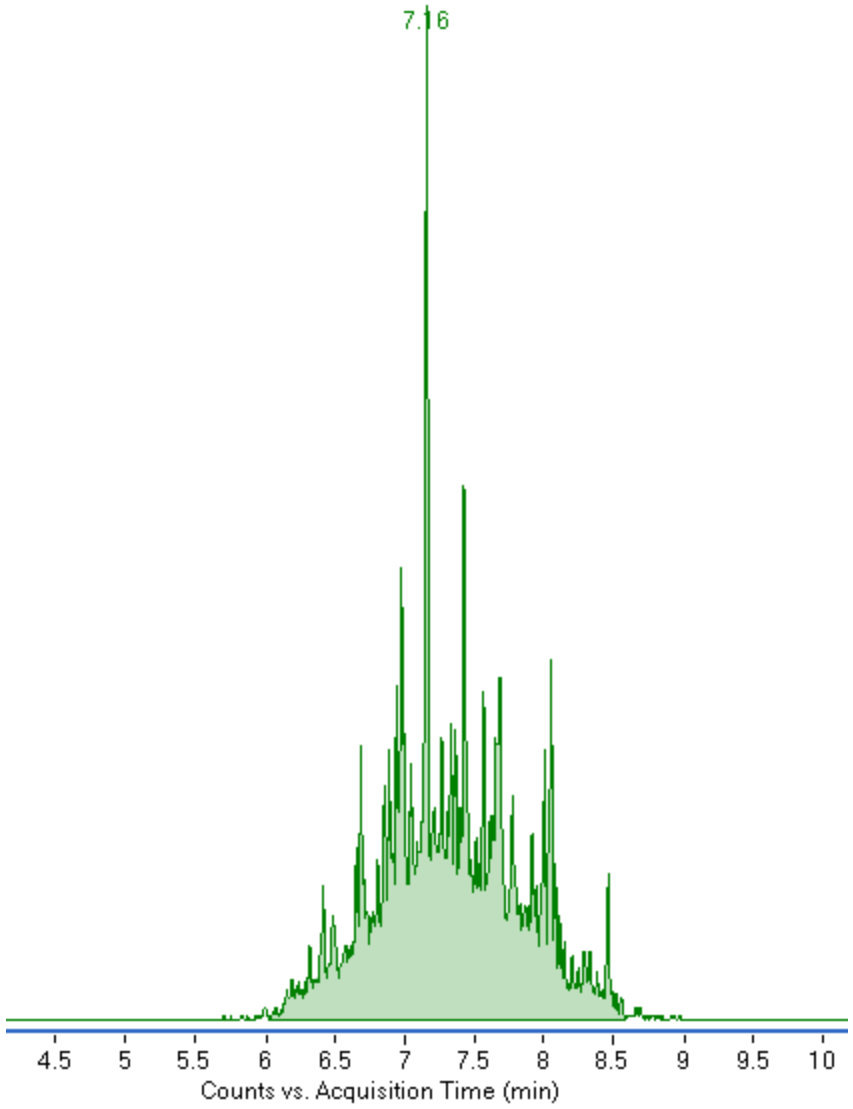
0.2 ng/ul Toxaphene Transition #1 293 → 257



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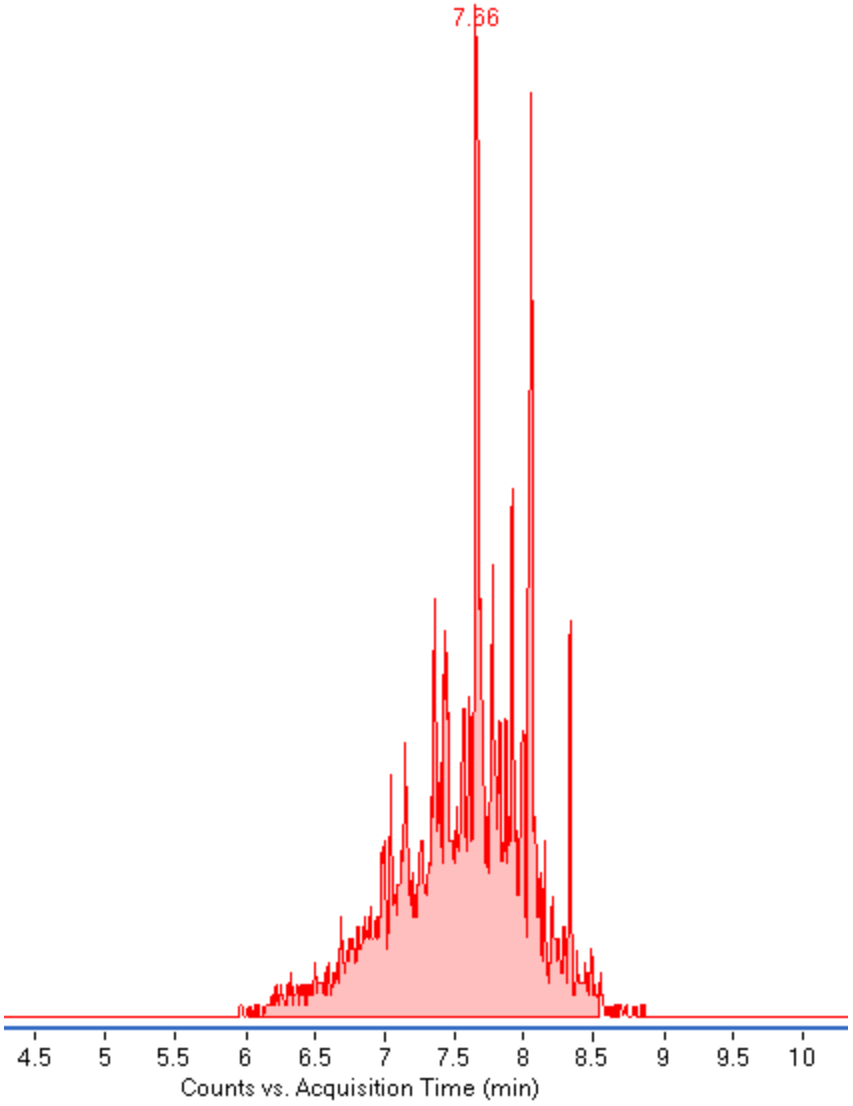
0.2 ng/ul Toxaphene Transition #2 341 → 305



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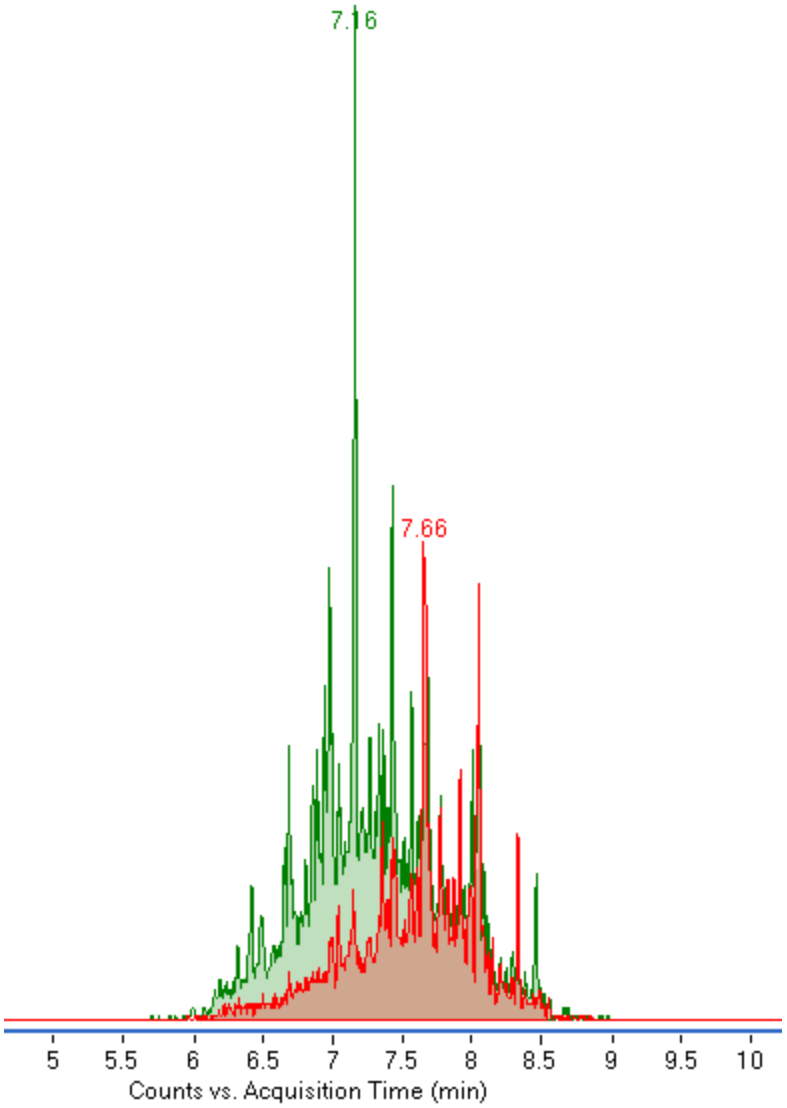
0.2 ng/ul Toxaphene Transition Overlay



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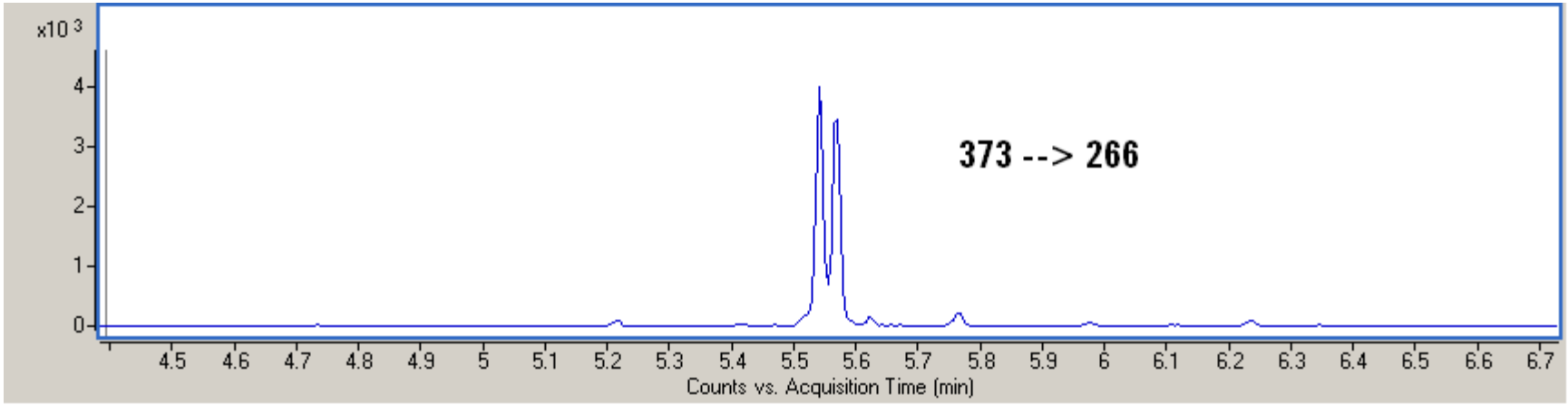
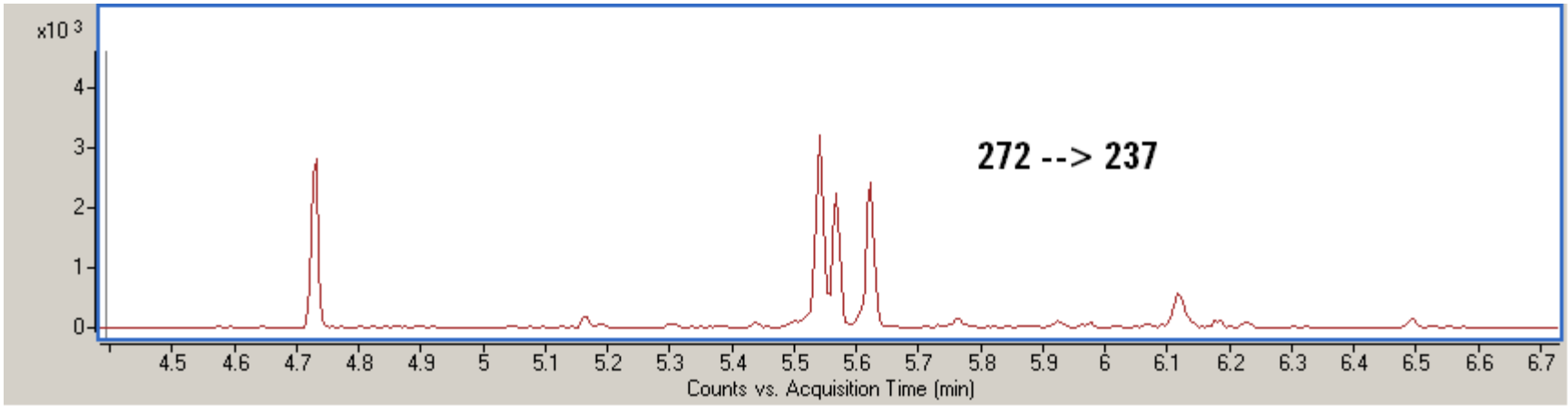
0.02 ng/ul Chlordane Transitions





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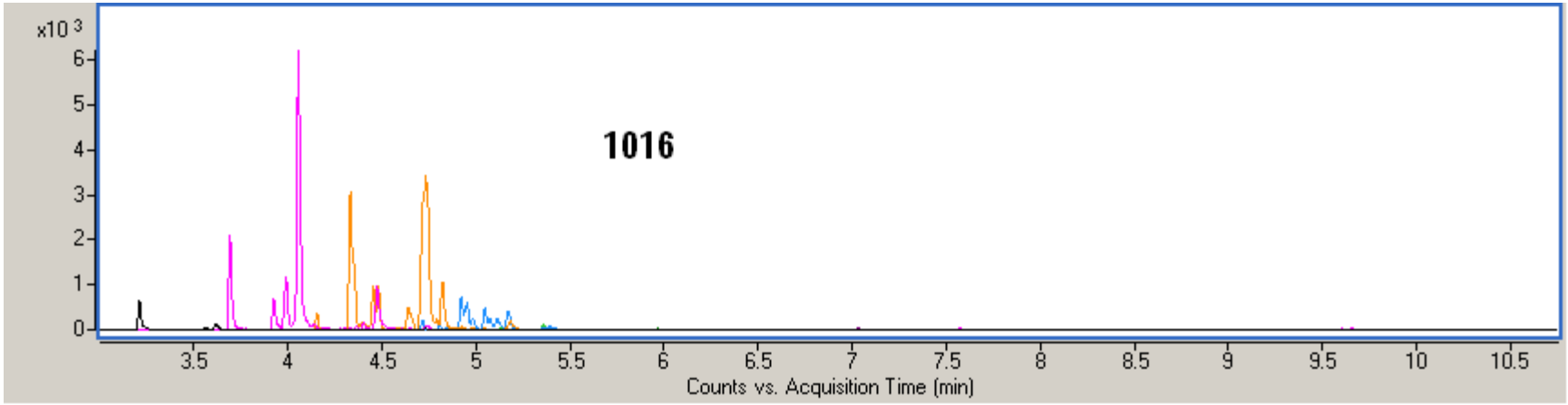
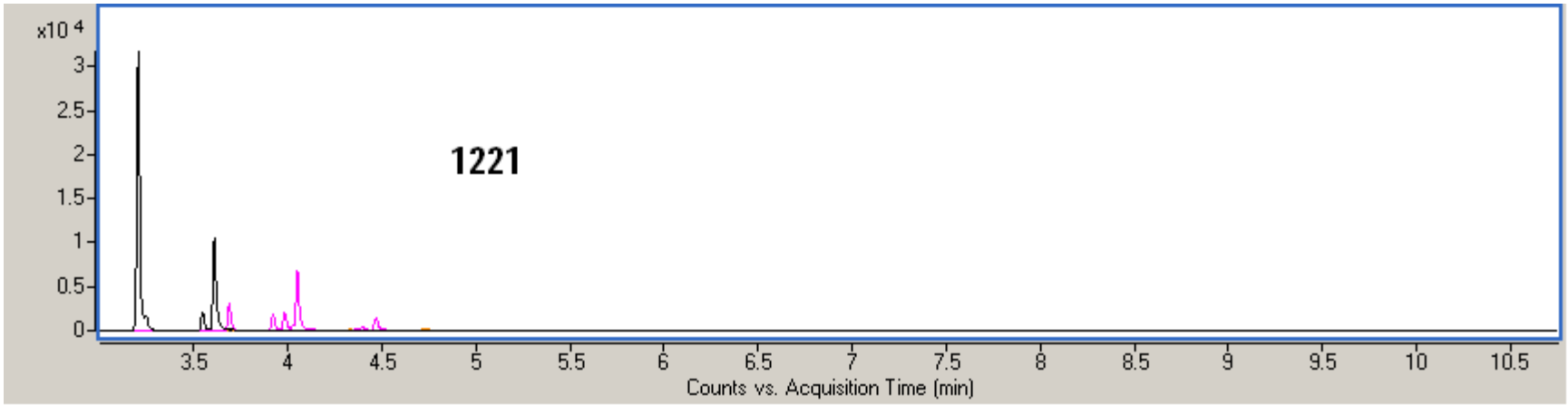
Arochlor Transitions 0.01 ng/ul





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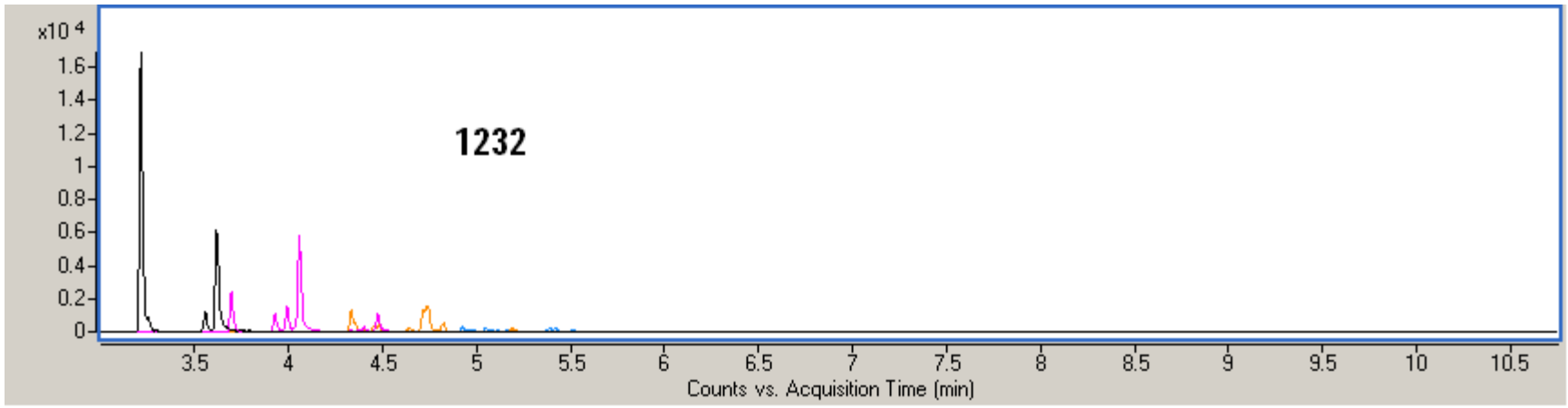
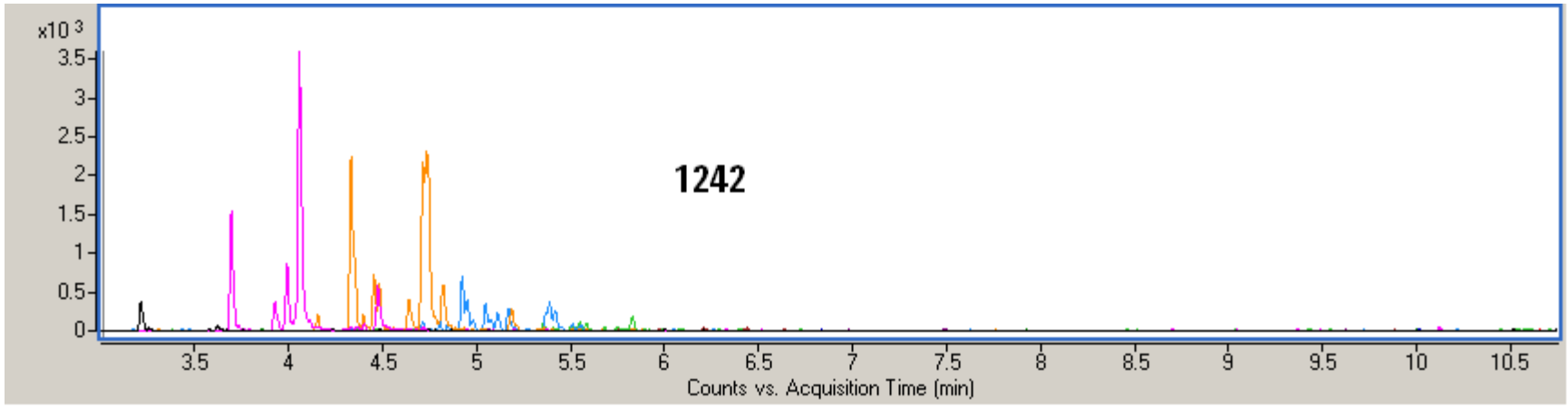
Arochlor Transitions 0.01 ng/ul





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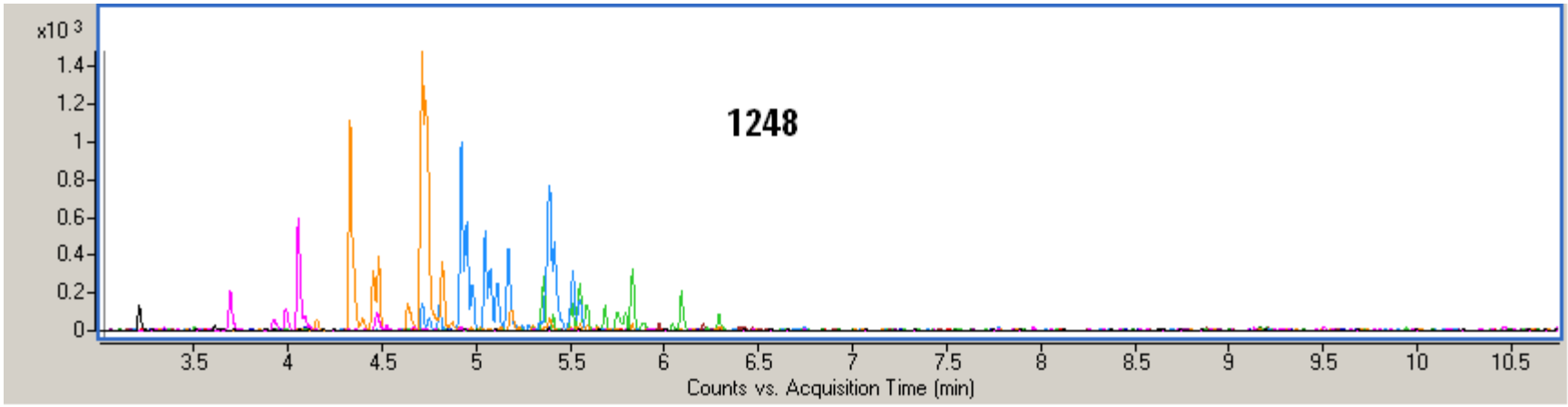
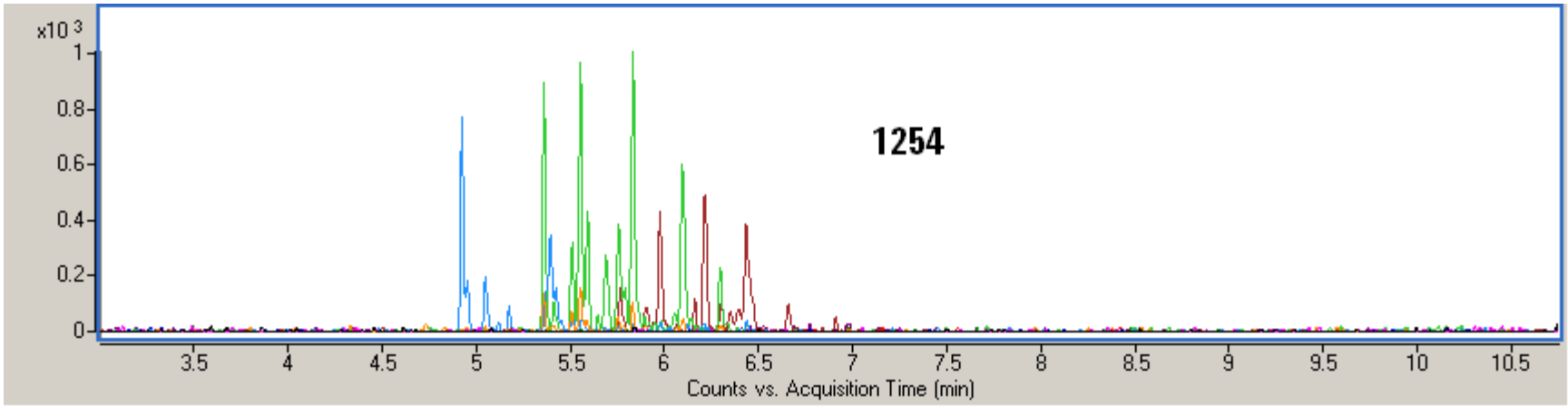
Arochlor Transitions 0.01 ng/ul





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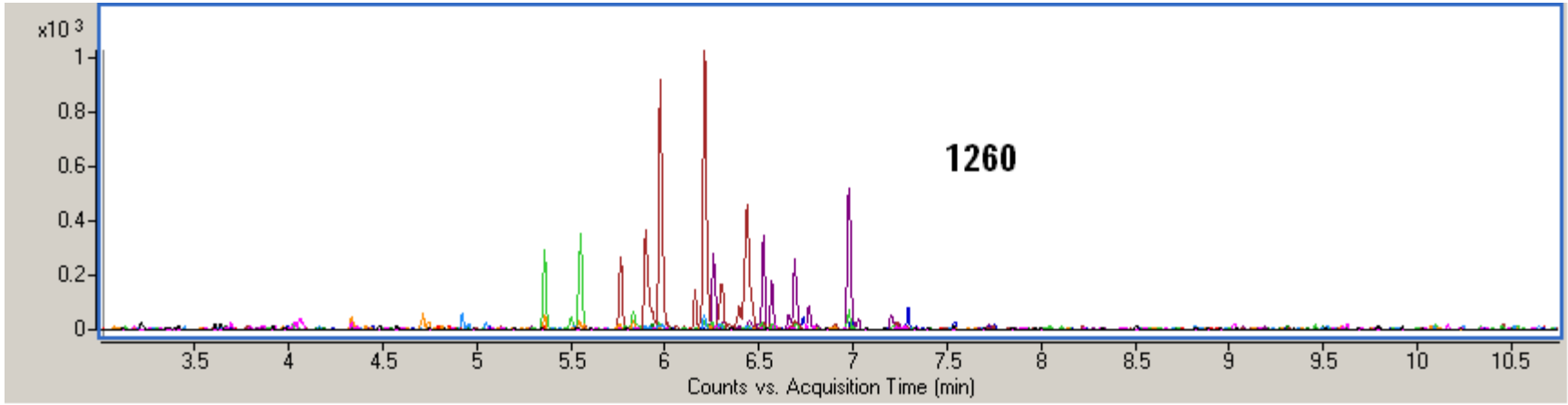
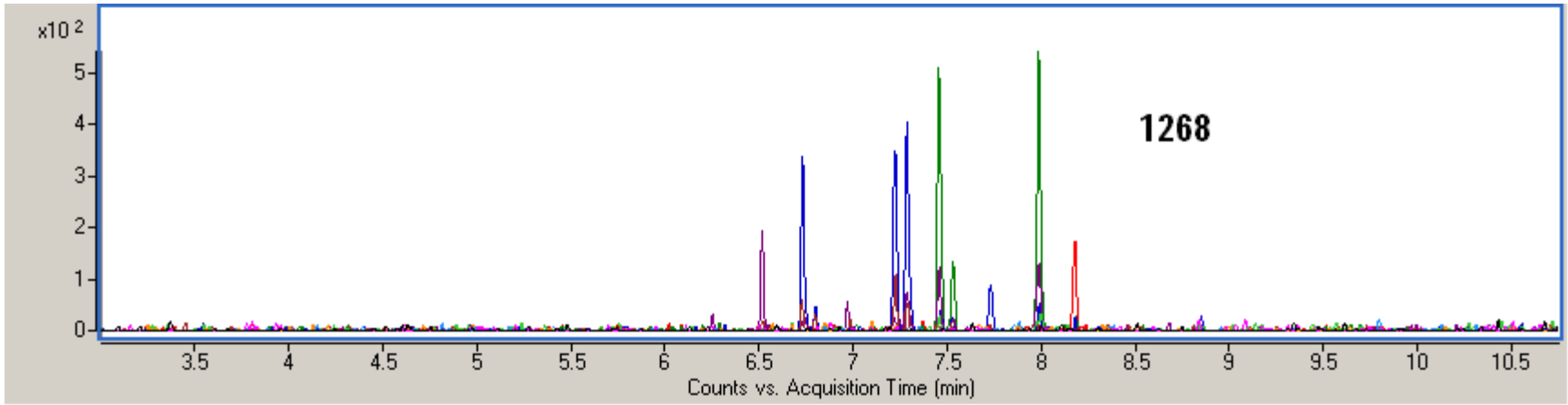
Arochlor Transitions 0.01 ng/ul





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Agilent MassHunter Quantitative Analysis - EPA Region IV - temp airochlor all plus tacoma

File Edit View Analyze Method Update Report Tools Help

Analyze Batch | Layout: | Restore Default Layout

Batch Table

Sample: 1232 ICA... | Sample Type: <All> | Compound: 1232 | ISTD:

Compound Group: <All> | Sample Group: <All> | ISTD: <All> | Time Segment: <All> | Sample/Compound Group: <All>

Sample							1232 Met...	1232 Results					Qualifier...		Qualifier...		Qualifier (...	
		Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Accuracy	Ratio	MI	Ratio	MI	Ratio	MI
		1016 ICAL 0.4 ppm 2012407	1016 ICAL CS5 2012407.D	Cal	1016-5	2/2/2012 9:13 AM		6.168	6460191		0.5618		1.7		161.6		43.4	
		1016 ICAL 0.2 ppm 2012406	1016 ICAL CS4 2012406.D	Cal	1016-4	2/2/2012 9:29 AM		6.168	2730485		0.2439		1.6		156.2		40.2	
		1016 ICAL 0.1 ppm 2012405	1016 ICAL CS3 2012405.D	Cal	1016-3	2/2/2012 9:45 AM		6.168	1301690		0.1222		1.6		158.0		39.4	
		1016 ICAL 0.05 ppm 2012404	1016 ICAL CS2 2012404.D	Cal	1016-2	2/2/2012 10:01 AM		6.168	612526		0.0635		1.6		156.1		40.2	
		1016 ICAL 0.025 ppm 2012403	1016 ICAL CS1 2012403.D	Cal	1016-1	2/2/2012 10:18 AM		6.168	277257		0.0349		2.0		153.2		37.6	
		1221 ICAL 0.4 ppm 2012412	1221 ICAL CS5 2012412.D	Cal	1221-5	2/2/2012 10:34 AM		6.168	5814787		0.5068		62.6		5.5		0.4	
		1221 ICAL 0.2 ppm 2012411	1221 ICAL CS4 2012411.D	Cal	1221-4	2/2/2012 10:50 AM		6.168	2776648		0.2479		62.3		5.4		0.5	
		1221 ICAL 0.05 ppm 2012409	1221 ICAL CS2 2012409.D	Cal	1221-2	2/2/2012 11:23 AM		6.168	655272		0.0671		60.6		5.2		0.5	
		1221 ICAL 0.025 ppm 2012408	1221 ICAL CS1 2012408.D	Cal	1221-1	2/2/2012 11:39 AM		6.168	317639		0.0383		62.2		5.5		0.6	
▶		1232 ICAL 0.4 ppm 2012417	1232 ICAL CS5 2012417.D	Cal	1232-5	2/2/2012 11:55 AM	0.4000	6.168	4670343		0.4093	102.3	44.5		42.5		8.4	
		1232 ICAL 0.2 ppm 2012416	1232 ICAL CS4 2012416.D	Cal	1232-4	2/2/2012 12:11 PM	0.2000	6.168	2062603		0.1870	93.5	43.3		43.4		9.1	
		1232 ICAL 0.1 ppm 2012415	1232 ICAL CS3 2012415.D	Cal	1232-3	2/2/2012 12:28 PM	0.1000	6.168	894648		0.0875	87.5	44.5		46.7		9.7	
		1232 ICAL 0.05 ppm 2012414	1232 ICAL CS2 2012414.D	Cal	1232-2	2/2/2012 12:44 PM	0.0500	6.168	462255		0.0507	101.3	44.1		45.2		8.8	
		1232 ICAL 0.025 ppm 2012413	1232 ICAL CS1 2012413.D	Cal	1232-1	2/2/2012 1:00 PM	0.0250	6.168	211770		0.0293	117.2	43.5		40.7		9.4	
		1242 ICAL 0.4 ppm 2012422	1242 ICAL CS5 2012422.D	Cal	1242-5	2/2/2012 1:16 PM		6.168	4011945		0.3532		1.7		152.9		38.9	
		1242 ICAL 0.2 ppm 2012421	1242 ICAL CS4 2012421.D	Cal	1242-4	2/2/2012 1:32 PM		6.168	1988394		0.1807		1.7		148.9		37.0	
		1242 ICAL 0.1 ppm 2012420	1242 ICAL CS3 2012420.D	Cal	1242-3	2/2/2012 1:49 PM		6.168	939287		0.0913		1.9		145.5		35.2	
		1242 ICAL 0.05 ppm 2012419	1242 ICAL CS2 2012419.D	Cal	1242-2	2/2/2012 2:05 PM		6.168	489190		0.0529		1.8		143.0		35.3	
		1242 ICAL 0.025 ppm 2012418	1242 ICAL CS1 2012418.D	Cal	1242-1	2/2/2012 2:21 PM		6.168	235012		0.0313		1.9		144.6		32.6	
		1248 ICAL 0.4 ppm 2012606	1248 ICAL CS5 2012606.D	Cal	1248-5	2/2/2012 2:37 PM		6.168	2674569		0.2392		3.3		458.9		377.0	
		1248 ICAL 0.2 ppm 201205	1248 ICAL CS4 201205.D	Cal	1248-4	2/2/2012 2:54 PM		6.168	1169025		0.1109		3.8		459.6		367.3	
		1248 ICAL 0.1 ppm 2012604	1248 ICAL CS3 2012604.D	Cal	1248-3	2/2/2012 3:10 PM		6.168	574236		0.0602		4.0		449.6		349.9	
		1248 ICAL 0.05 ppm 2012603	1248 ICAL CS2 2012603.D	Cal	1248-2	2/2/2012 3:26 PM		6.168	278080		0.0350		2.6		443.7		351.0	
		1248 ICAL 0.025 ppm 2012602	1248 ICAL CS1 2012602.D	Cal	1248-1	2/2/2012 3:42 PM		6.168	160073		0.0249		4.9		467.8		360.6	
		1254 ICAL 0.4 ppm 2012611	1254 ICAL CS5 2012611.D	Cal	1254-5	2/2/2012 3:58 PM		6.168	352243		0.0413		11.0		264.8		3642.1	
		1254 ICAL 0.2 ppm 2012610	1254 ICAL CS4 2012610.D	Cal	1254-4	2/2/2012 4:15 PM		6.168	169664		0.0257		9.4		220.7		2971.4	
		1254 ICAL 0.1 ppm 2012609	1254 ICAL CS3 2012609.D	Cal	1254-3	2/2/2012 4:31 PM		6.168	102100		0.0200		17.5		243.6		3174.9	
		1254 ICAL 0.05 ppm 2012608	1254 ICAL CS2 2012608.D	Cal	1254-2	2/2/2012 4:47 PM		6.168	47355		0.0153		16.5		212.8		2339.2	
		1254 ICAL 0.025 ppm 2012607	1254 ICAL CS1 2012607.D	Cal	1254-1	2/2/2012 5:03 PM		6.168	22652		0.0132		47.5		158.1		2491.7	
		1260 ICAL 0.4 ppm 2012616	1260 ICAL CS5 2012616.D	Cal	1260-5	2/2/2012 5:19 PM		6.168	48935		0.0154		9.0		124.9		87.7	
		1260 ICAL 0.2 ppm 2012615	1260 ICAL CS4 2012615.D	Cal	1260-4	2/2/2012 5:36 PM		6.168	22863		0.0132		8.5		126.1		91.3	
		1260 ICAL 0.1 ppm 2012614	1260 ICAL CS3 2012614.D	Cal	1260-3	2/2/2012 5:52 PM		6.168	11170		0.0122		14.2		120.4		71.5	

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Details of Arochlor Identification and Quantitation

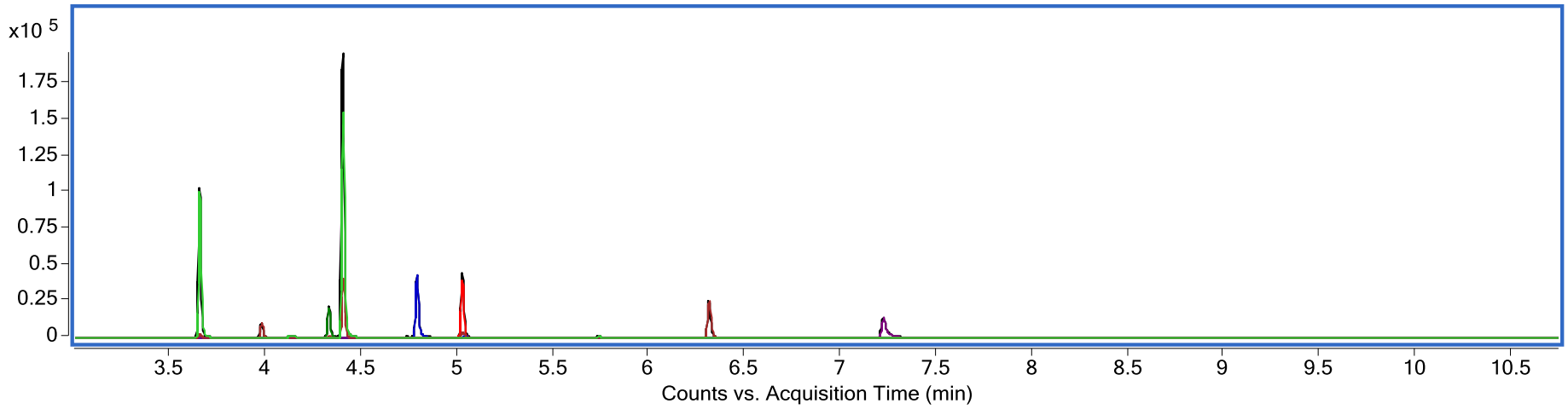
- These were covered in a previous eSeminar by Dale Walker
- Recording of this seminar is available at Agilent.com
- Simply put “Dale Walker” in the search box

EPA Method 8141

- **Organophosphorus Pesticides by GC/NPD or FPD**
- **Easily met detection limit requirements**

OP Pesticide Transitions 0.1 ng/ul

Name	TS	Transition	Scan	Type
Carbophenothion	1	153.0 -> 96.9	MRM	Target
Chlorpyrifos	1	313.8 -> 258.0	MRM	Target
Diazinon	1	304.0 -> 179.0	MRM	Target
disuloton	1	88.1 -> 60.0	MRM	Target
Guthion	1	160.1 -> 77.1	MRM	Target
Methyl Parathion	1	263.0 -> 109.1	MRM	Target



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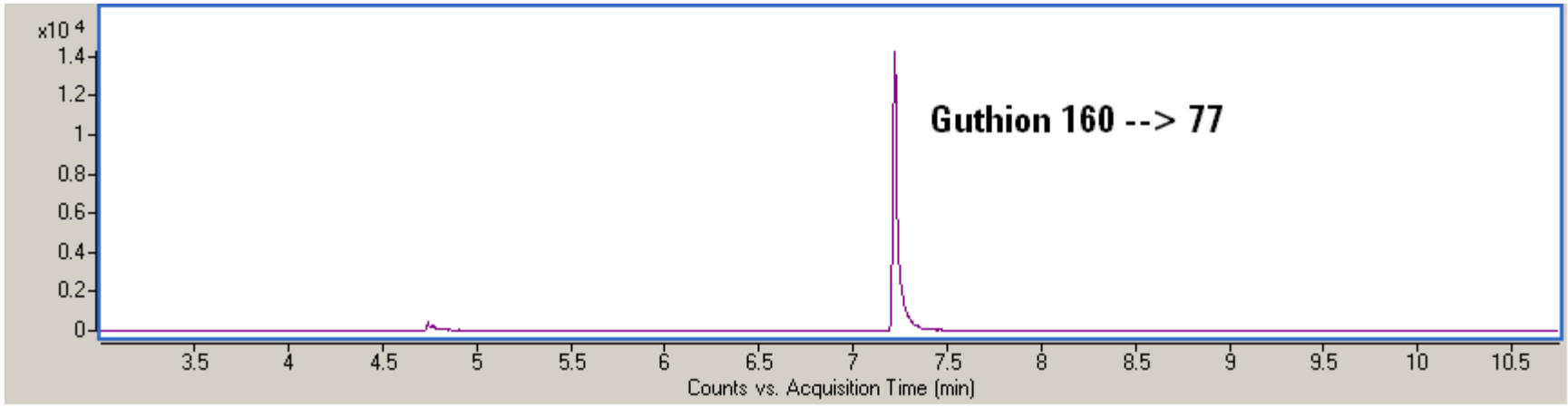
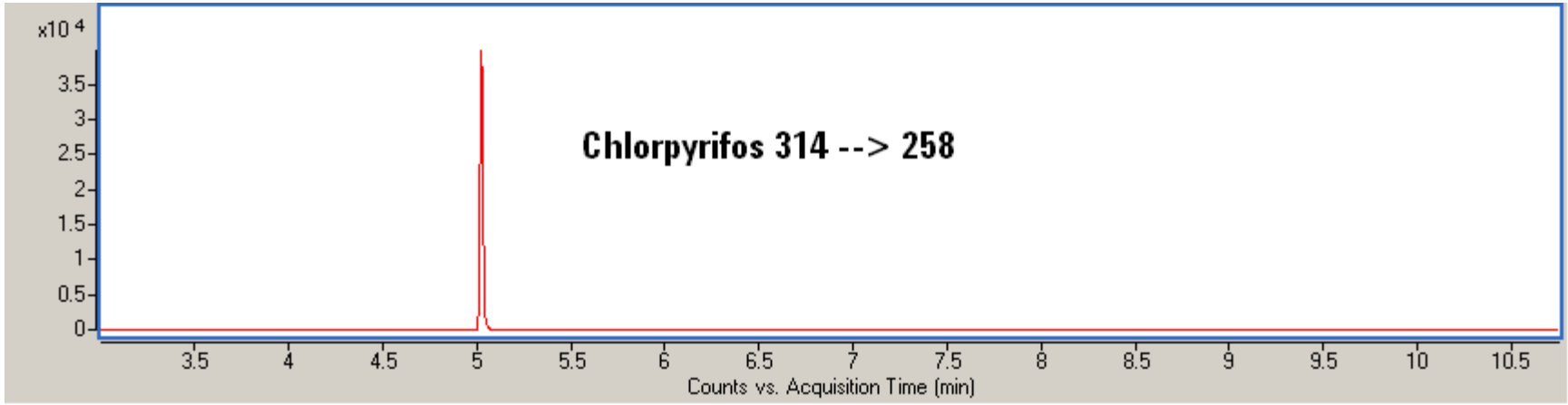
OP Pesticide Transitions 0.1 ng/ul





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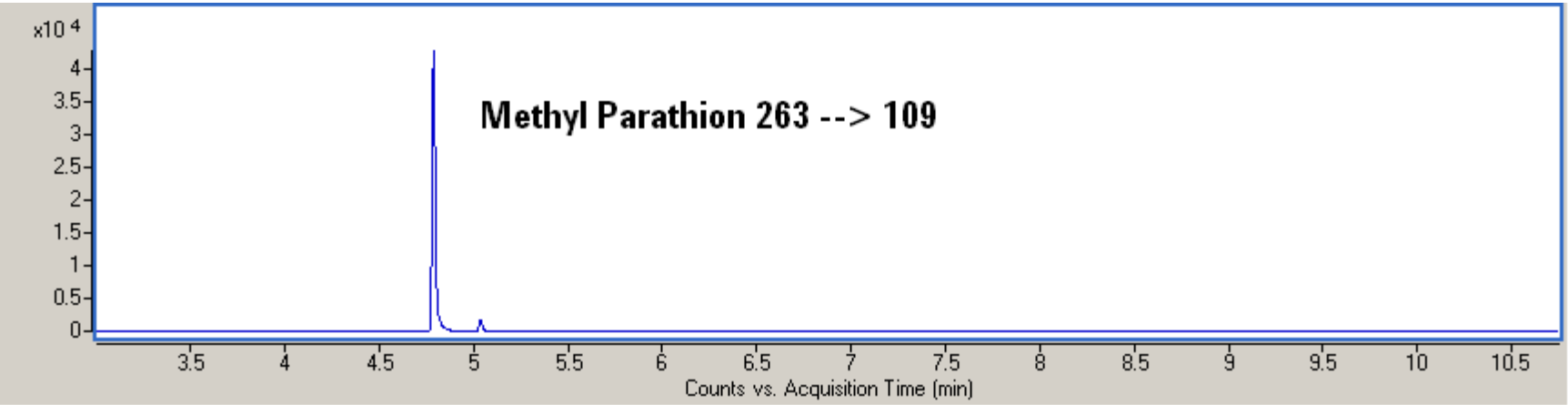
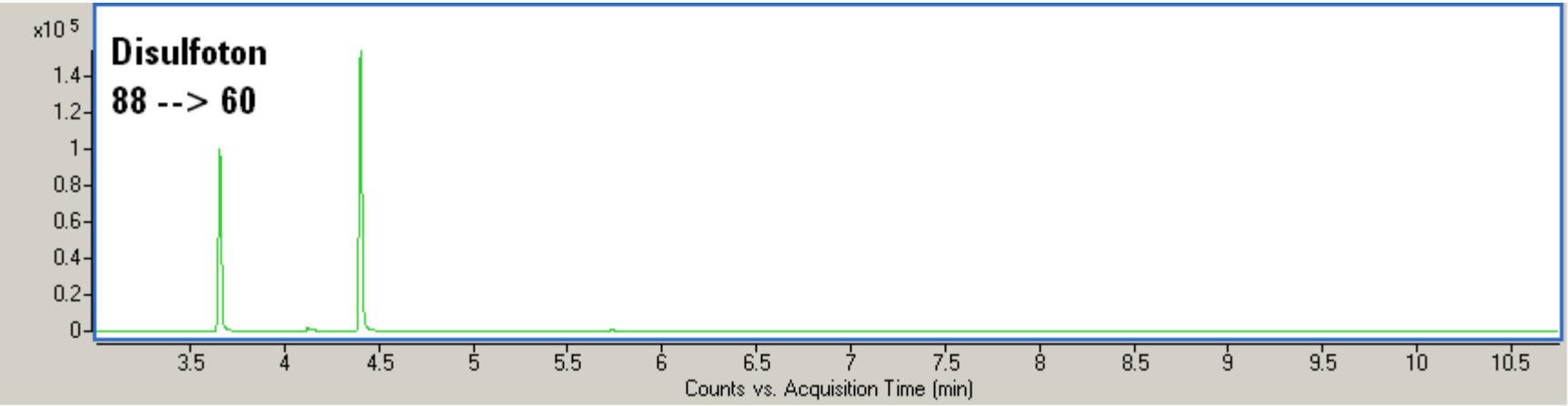
OP Pesticide Transitions 0.1 ng/ul





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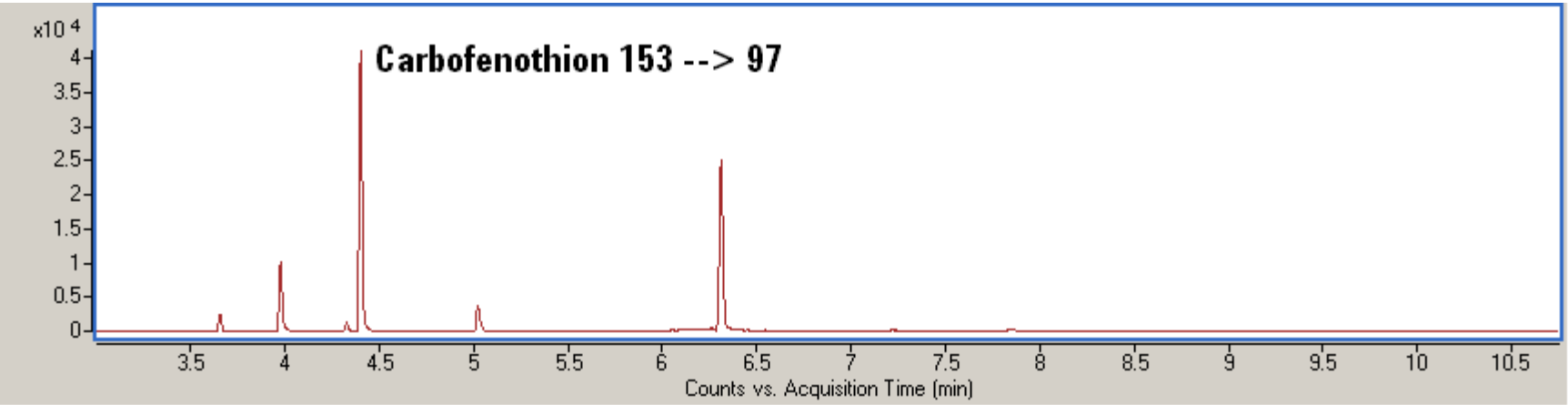
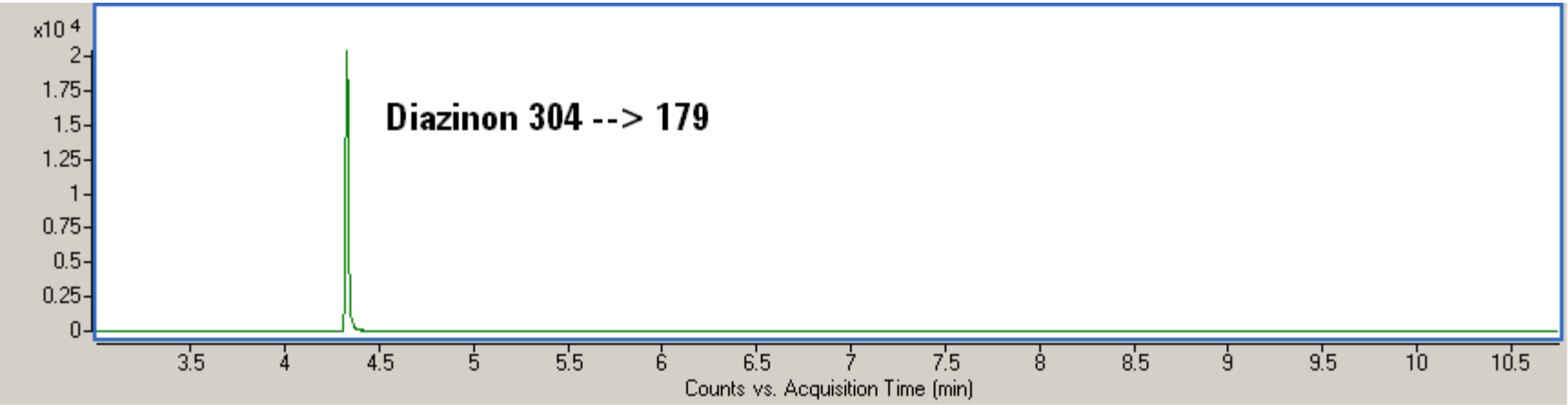
OP Pesticide Transitions 0.1 ng/ul





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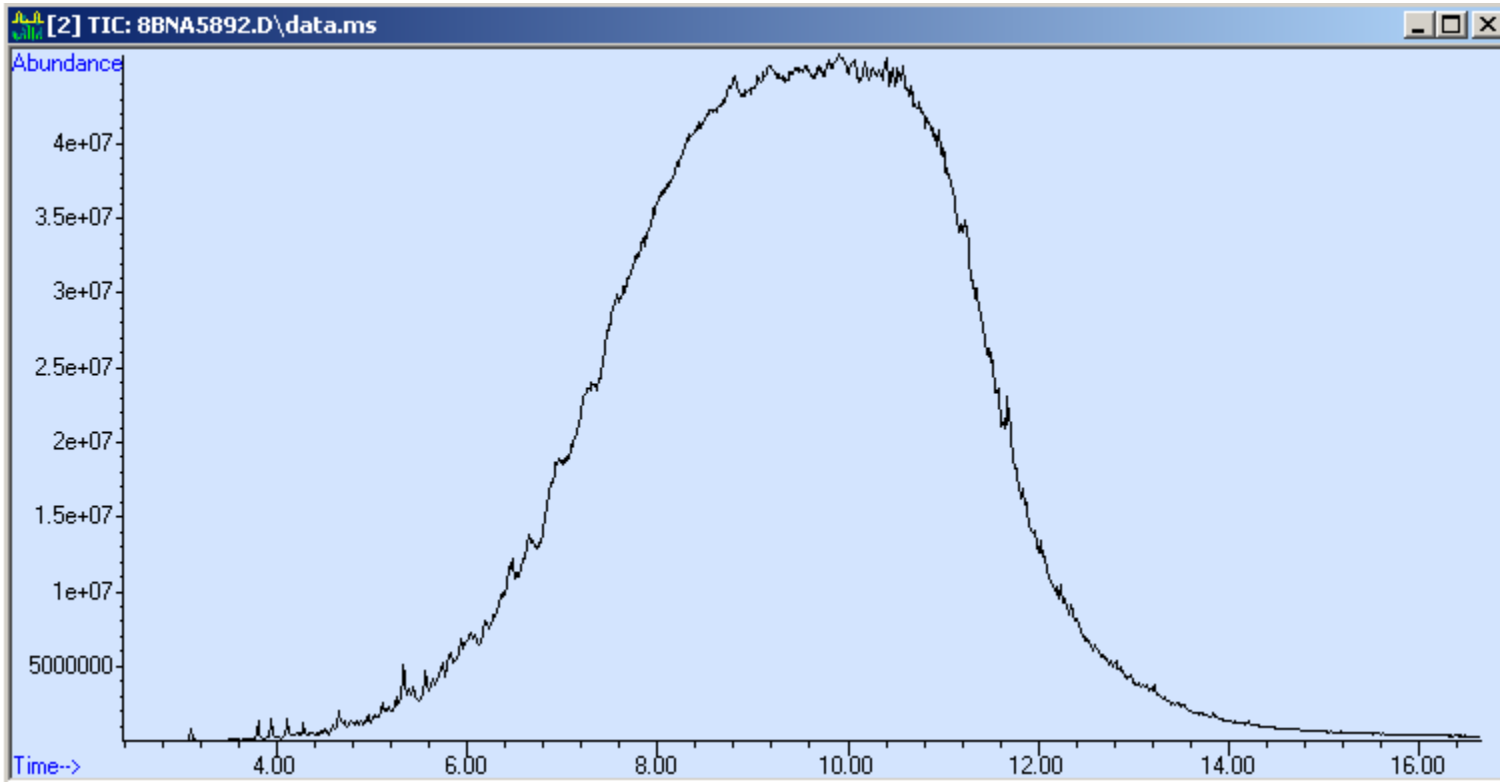
EPA Method 8270

- EPA methods are detector specific
  - If using a MS, by definition you are doing method 8270
- This means:
  - 8270 Internal standards and surrogates
  - Meet all QC requirements
  - Initial calibration and continuing calibration checks
  - DFTPP tuning?
    - Still under discussion with EPA
    - 8270 allows tune criteria from manufacturer

EPA Method 8270 on GC-QQQ

- For now, we only look for targeted compound groups
  - Not the full 8270 list
- Why?
  - The MSD single quad is the workhorse for general 8270 analysis
  - The QQQ is used when interference problems arise
  - The QQQ is used when lower detection levels are needed
- The QQQ can also speed up data review and total analysis times

8270 Soil Extract – Challenging matrix



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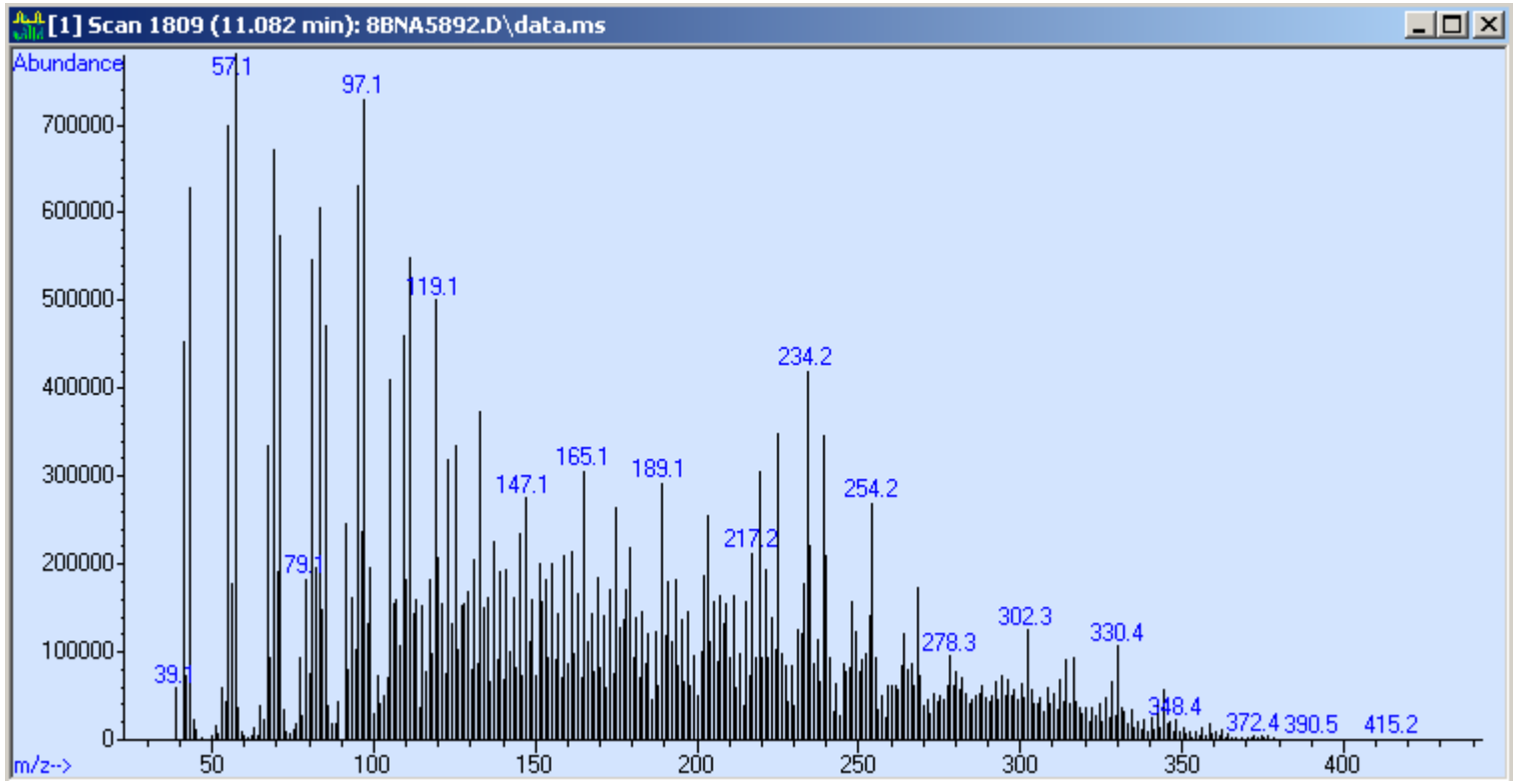
Typical spectrum from oil laden soil extract



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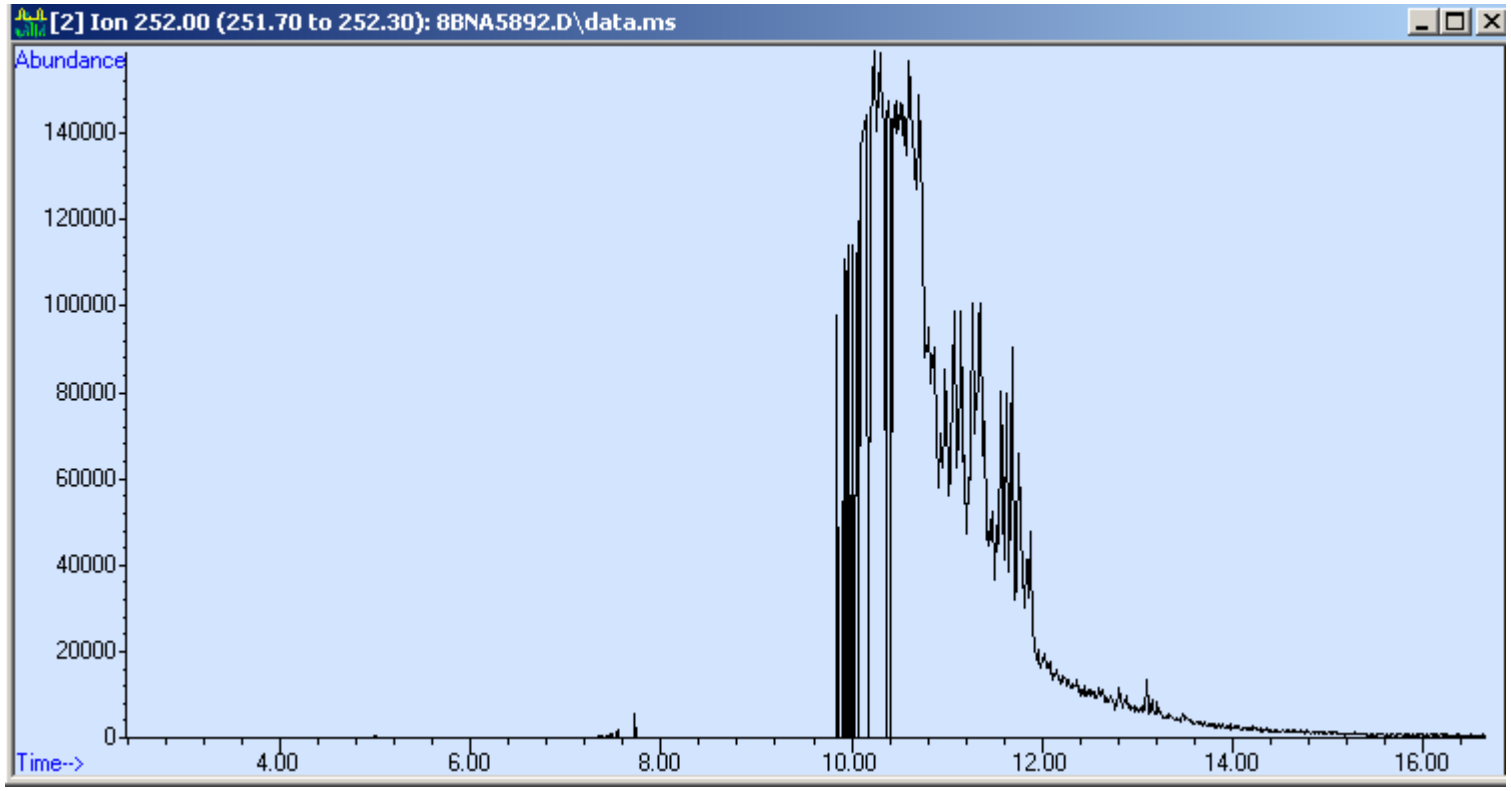
Benzo(a)pyrene?
Extract primary ion: 252
Result inconclusive



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Course of Action

- **Based on MSD single quad data, suspect PAH contamination**
- **Only interested in 8270 regulated PAH's**
- **Set up GC-QQQ for targeted PAH analysis following 8270 guidelines**
  - **ISTD's and Surrogates**
  - **Meet QC Requirements**
- **Prepare for low level (< 1.0 ppm) detection in complex matrix**
- **Calibration range desired: 1.0 pg/ul – 1000 pg/ul (ng/ml)**

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

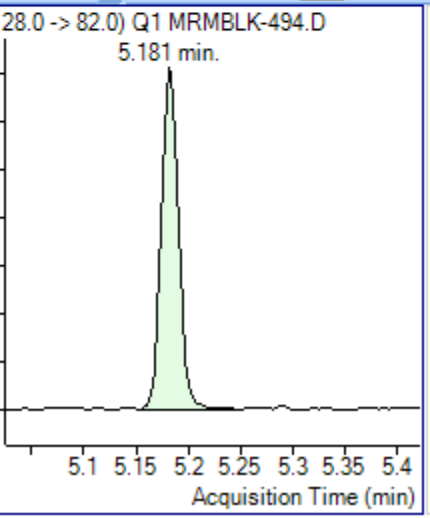
Analyze Batch | Layout: | Restore Default Layout

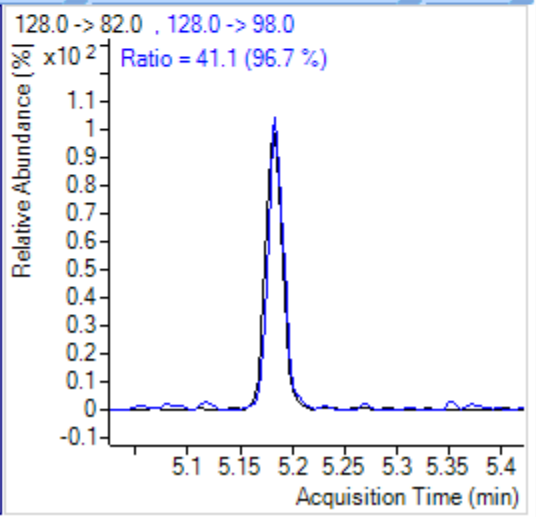
le

le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: Nitrobenzene-d5 | ISTD: Naph

Sample					Nitrobenz...	Nitrobenzene-d5 Results						Qualifier...	Nap
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	5.181	163		1.0641	1.0641	106.4	41.1		5.88
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	5.181	303		2.1436	2.1436	107.2	44.5		5.88
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	5.181	602		4.1801	4.1801	104.5	41.6		5.88
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	5.184	1495		9.5957	9.5957	96.0	42.8		5.88
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	5.181	2739		19.2314	19.2314	96.2	42.4		5.88
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	5.181	6331		47.4756	47.4756	95.0	42.5		5.88
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	5.181	13543		98.5108	98.5108	98.5	42.4		5.88
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	5.181	22876		191.5868	191.5868	95.8	42.2		5.88
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	5.181	58475		394.9164	394.9164	98.7	42.2		5.88
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	5.181	116815		799.2884	799.2884	99.9	42.2		5.88
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	5.181	141755		1019.0072	1019.0072	101.9	42.7		5.88
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		5.181	11399		75.0426	75.0426		42.3		5.88

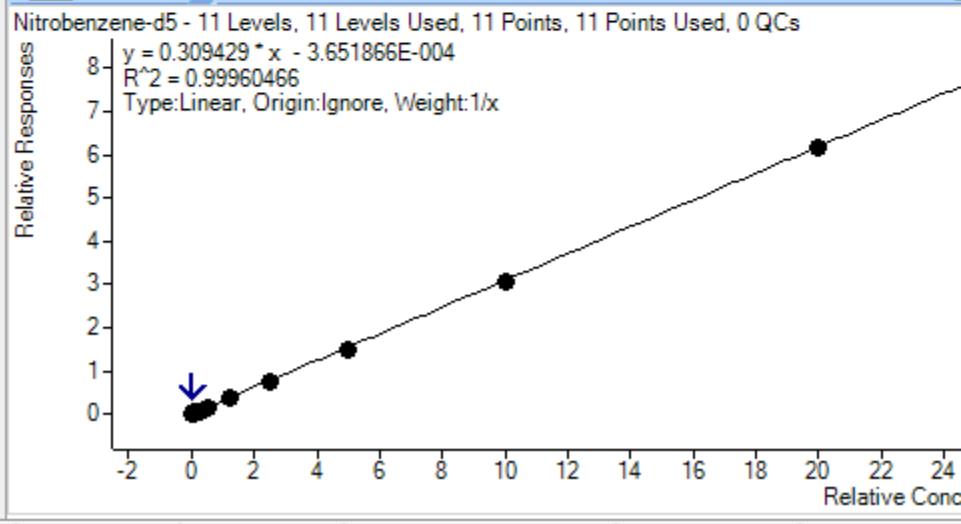
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1.0 ng/ml QQQ PAH STD | Nitrobenzene-d5 | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

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Analyze Batch | Layout: | Restore Default Layout

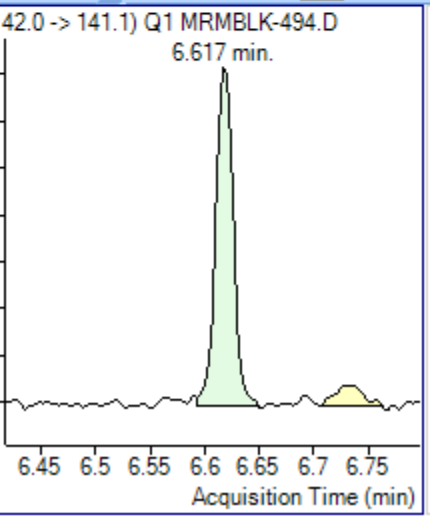
ple

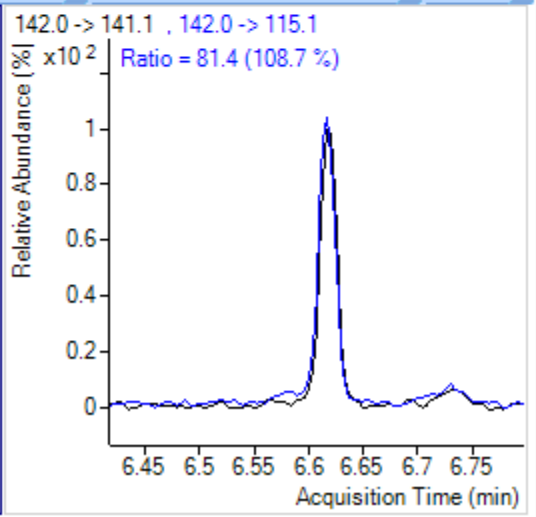
le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: 2-methyl naphthalene | ISTD: Naph

Worktable.Label.Compound

Sample					2-methyl naphthalene Results							Qualifier...	Nap
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	6.617	1613		0.5241	0.5241	52.4	81.4		5.88
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	6.617	2944		2.2245	2.2245	111.2	75.8		5.88
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	6.617	5636		5.2427	5.2427	131.1	73.7		5.88
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	6.617	11223		10.6782	10.6782	106.8	74.7		5.88
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	6.617	18482		20.2047	20.2047	101.0	75.1		5.88
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	6.617	41455		50.0660	50.0660	100.1	74.9		5.88
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	6.617	84330		99.9428	99.9428	99.9	74.7		5.88
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	6.617	142164		195.1062	195.1062	97.6	74.6		5.88
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	6.617	358526		397.9997	397.9997	99.5	74.8		5.88
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	6.617	705427		794.5684	794.5684	99.3	74.8		5.88
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	6.617	853614		1010.4427	1010.4427	101.0	74.9		5.88
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		6.617	70093		74.8874	74.8874		74.1		5.88

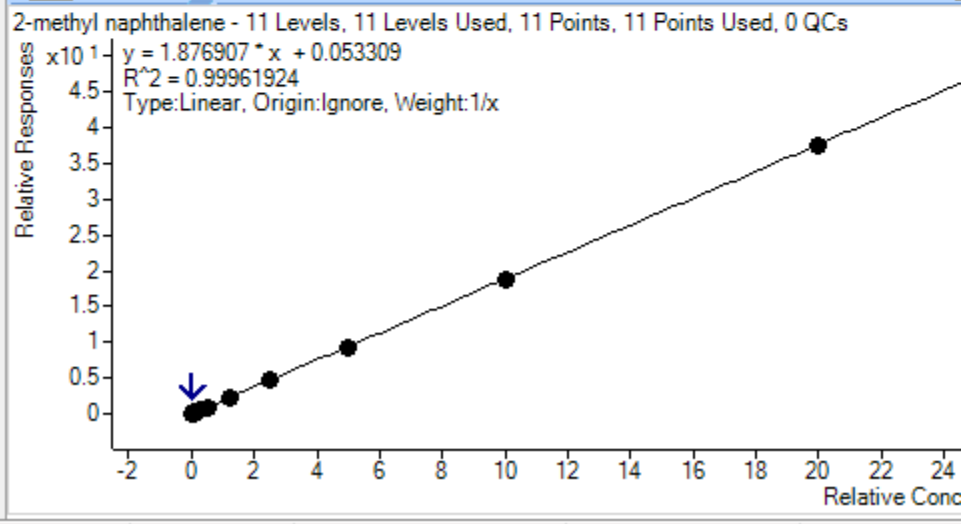
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1.0 ng/ml QQQ PAH STD | 2-methyl naphthalene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

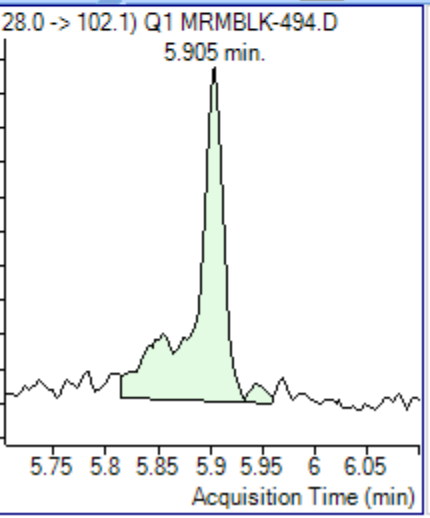
Analyze Batch | Layout: | Restore Default Layout

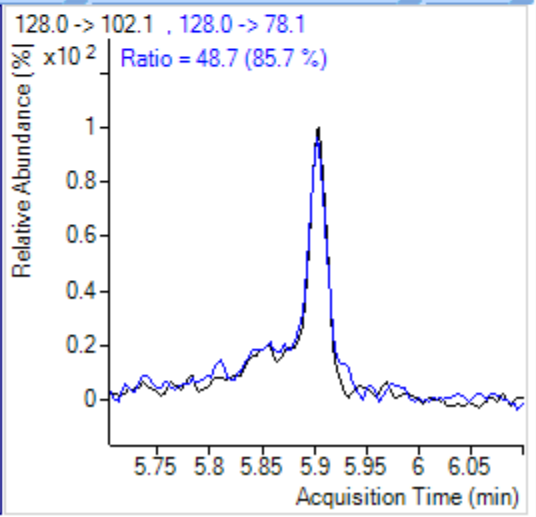
le

le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: Naphthalene | ISTD: Naph

Sample					Naphthale...	Naphthalene Results					Qualifier...	Nap
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	5.905	1895		0.9506	0.9506	95.1	48.7		5.88
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	5.905	2383		2.2859	2.2859	114.3	44.4		5.88
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	5.905	3227		3.9027	3.9027	97.6	59.4		5.88
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	5.905	6625		9.6704	9.6704	96.7	56.8		5.88
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	5.905	11101		19.8132	19.8132	99.1	57.0		5.88
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	5.905	24143		49.3237	49.3237	98.6	56.9		5.88
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	5.905	49426		100.3962	100.3962	100.4	57.3		5.88
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	5.905	82991		196.4145	196.4145	98.2	56.9		5.88
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	5.905	207541		398.6132	398.6132	99.7	57.0		5.88
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	5.905	406513		793.4825	793.4825	99.2	57.2		5.88
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	5.905	493237		1012.1470	1012.1470	101.2	57.1		5.88
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		5.905	28901		51.9733	51.9733		57.2		5.88

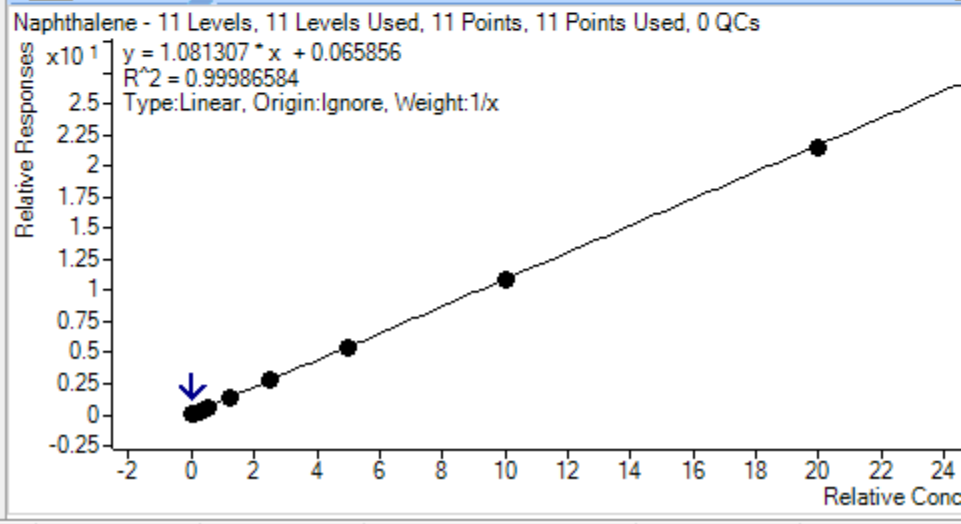
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1.0 ng/ml QQQ PAH STD | Naphthalene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

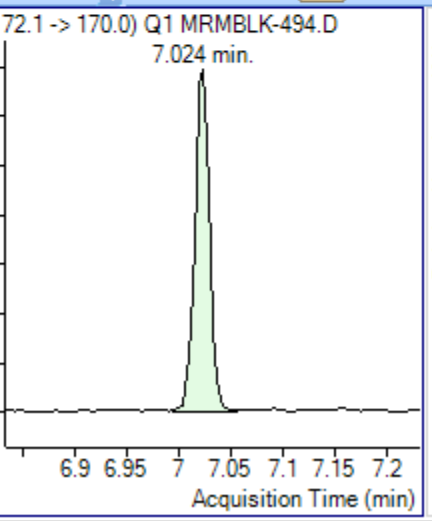
Analyze Batch | Layout: | Restore Default Layout

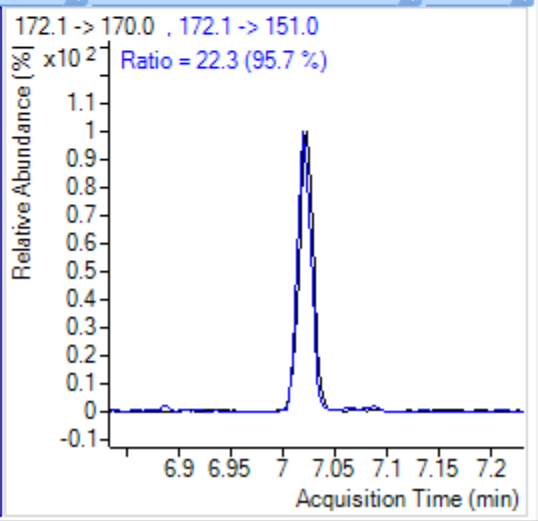
ble

le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: 2-Fluorobiphenyl | ISTD: Acen

Sample					2-Fluorobi...	2-Fluorobiphenyl Results					Qualifier...	Acer
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	7.024	338		0.5140	0.5140	51.4	22.3		7.73
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	7.024	644		2.3020	2.3020	115.1	24.0		7.73
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	7.020	1237		5.2672	5.2672	131.7	22.3		7.73
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	7.024	2484		10.6150	10.6150	106.1	22.5		7.73
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	7.024	4075		19.9894	19.9894	99.9	23.4		7.73
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	7.024	9139		48.9945	48.9945	98.0	23.4		7.73
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	7.020	18504		100.4494	100.4494	100.4	23.1		7.73
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	7.024	31261		195.3357	195.3357	97.7	23.0		7.73
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	7.024	78476		395.7490	395.7490	98.9	23.1		7.73
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	7.024	155278		796.0488	796.0488	99.5	23.1		7.73
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	7.024	187565		1011.7351	1011.7351	101.2	23.3		7.73
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		7.024	14519		70.7434	70.7434		23.2		7.73

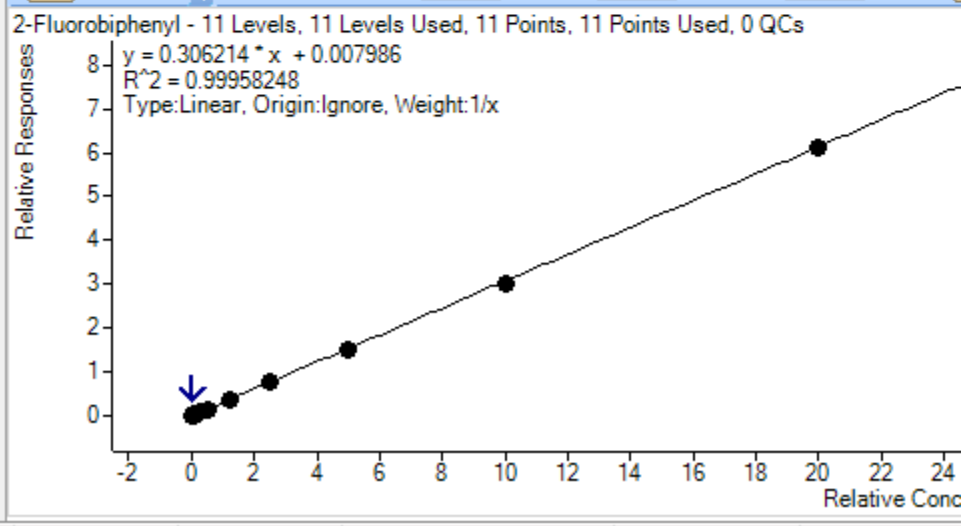
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1.0 ng/ml QQQ PAH STD | 2-Fluorobiphenyl | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

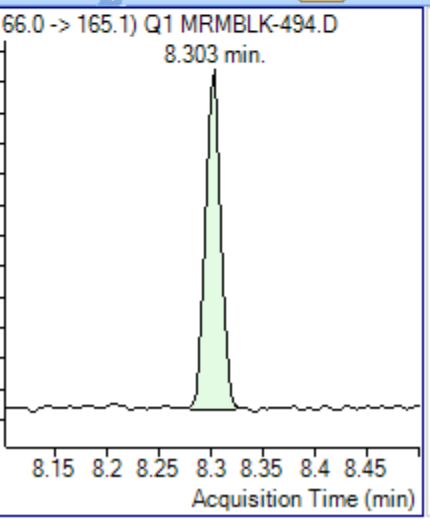
Analyze Batch | Layout: | Restore Default Layout

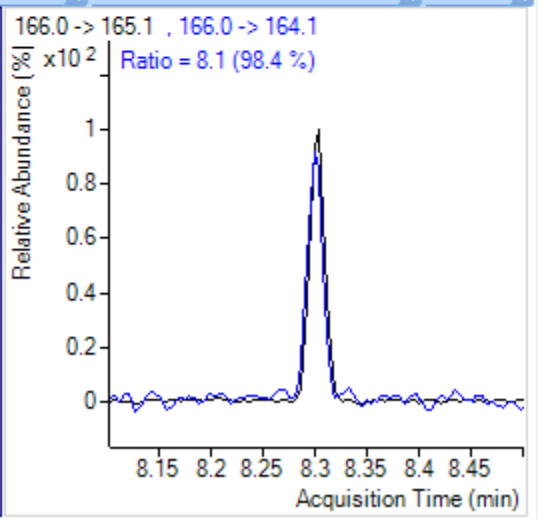
ple

le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: Fluorene | ISTD: Acen

Sample					Fluorene...	Fluorene Results					Qualifier...	Acer
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	8.303	2793		0.4356	0.4356	43.6	8.1		7.73
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	8.303	4556		2.3053	2.3053	115.3	8.7		7.73
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	8.303	7933		5.2080	5.2080	130.2	8.5		7.73
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	8.303	16424		11.5352	11.5352	115.4	8.2		7.73
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	8.303	24268		19.8553	19.8553	99.3	8.1		7.73
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	8.303	54497		49.7716	49.7716	99.5	8.2		7.73
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	8.303	106995		99.6161	99.6161	99.6	8.2		7.73
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	8.303	181211		194.9111	194.9111	97.5	8.2		7.73
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	8.303	455825		396.4576	396.4576	99.1	8.2		7.73
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	8.303	900713		797.1462	797.1462	99.6	8.2		7.73
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	8.303	10841...		1009.7579	1009.7579	101.0	8.2		7.73
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		8.306	72169		59.8724	59.8724		8.8		7.73

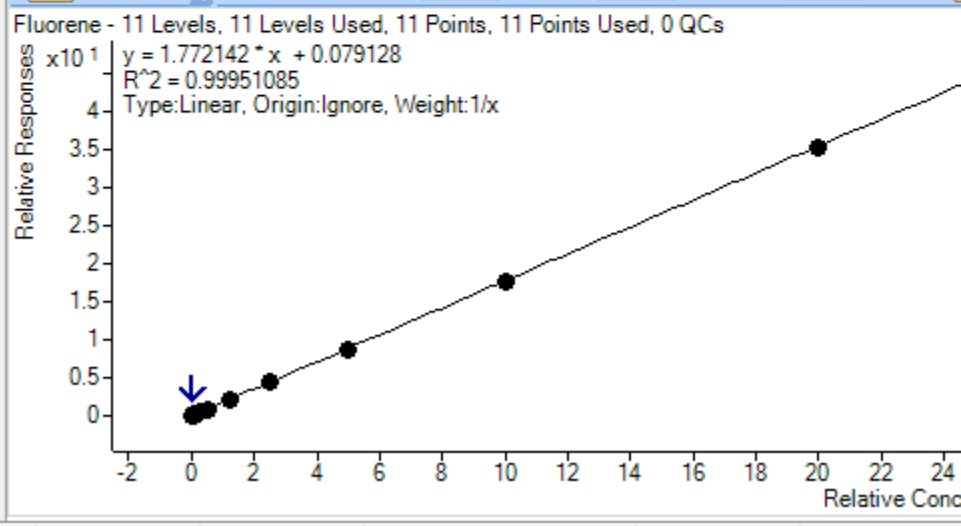
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1.0 ng/ml QQQ PAH STD | Fluorene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

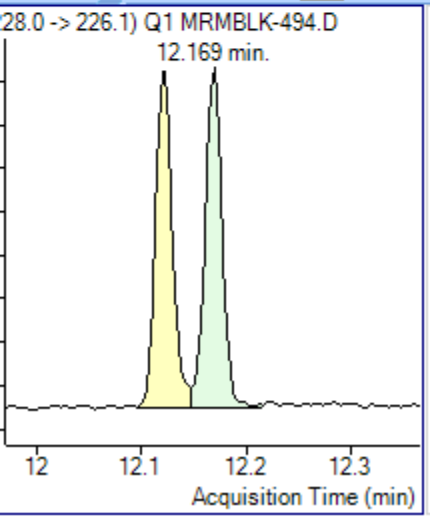
Analyze Batch | Layout: | Restore Default Layout

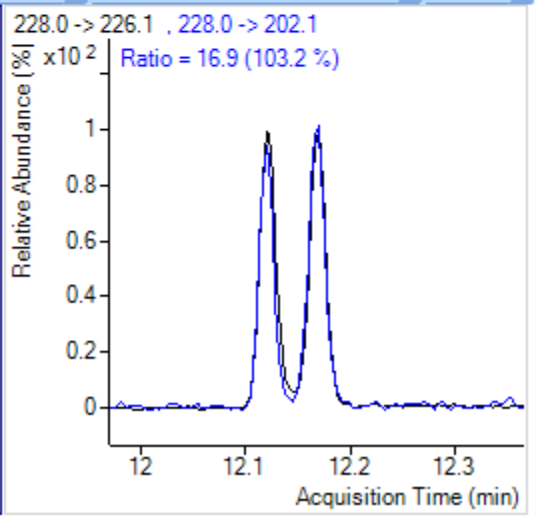
le

le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: Chrysene | ISTD: Chrys

Sample					Chrysene...	Chrysene Results					Qualifier...	Chry
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	12.1...	4426		0.5464	0.5464	54.6	16.9		12.1
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	12.1...	7042		2.3172	2.3172	115.9	17.5		12.1
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	12.1...	12571		5.4045	5.4045	135.1	17.2		12.1
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	12.1...	24497		10.4187	10.4187	104.2	16.5		12.1
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	12.1...	38520		19.3870	19.3870	96.9	16.8		12.1
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	12.1...	90356		49.1756	49.1756	98.4	16.4		12.1
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	12.1...	175468		98.5476	98.5476	98.5	16.5		12.1
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	12.1...	301568		196.9940	196.9940	98.5	16.7		12.1
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	12.1...	776179		384.8708	384.8708	96.2	16.7		12.1
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	12.1...	15210...		788.7921	788.7921	98.6	16.8		12.1
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	12.1...	18239...		1030.5463	1030.5463	103.1	16.9		12.1
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		12.2...	16636...	✓	676.2601	676.2601		13.7		12.1

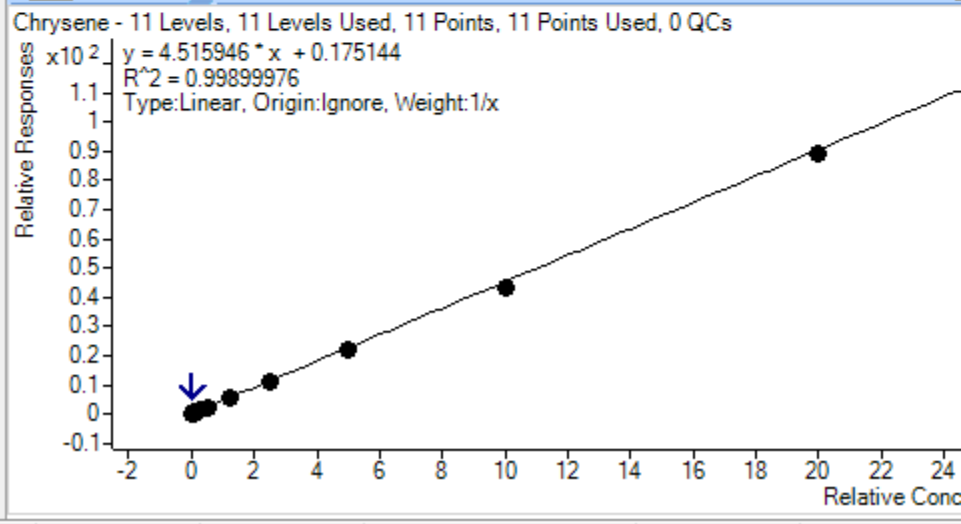
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1.0 ng/ml QQQ PAH STD | Chrysene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

Analyze Batch | Layout: | Restore Default Layout

le

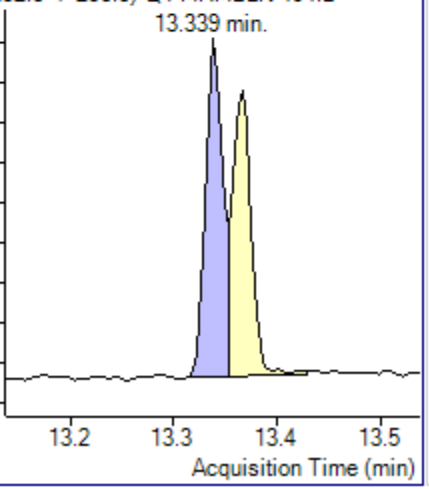
le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: Benzo (B) fluoranthene | ISTD: Peryl

Next Compound (Alt+Right)

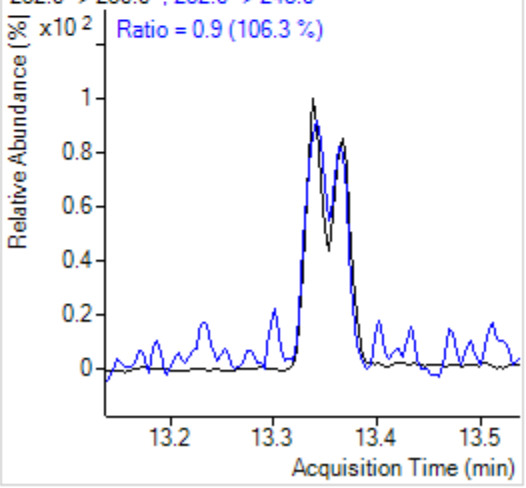
Sample					Benzo (B)...	Benzo (B) flu					Qualifier...	Pery
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	13.3...	4770		0.7283	0.7283	72.8	0.9		13.7
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	13.3...	7252		2.2852	2.2852	114.3	1.4		13.7
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	13.3...	12737		5.0323	5.0323	125.8	0.9		13.7
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	13.3...	25650		10.2316	10.2316	102.3	0.9		13.7
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	13.3...	40852		19.3694	19.3694	96.8	0.9		13.7
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	13.3...	91818		47.4792	47.4792	95.0	0.9		13.7
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	13.3...	188790		98.9966	98.9966	99.0	0.7		13.7
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	13.3...	321633		191.8873	191.8873	95.9	0.8		13.7
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	13.3...	828761		378.6238	378.6238	94.7	0.8		13.7
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	13.3...	16593...		806.0455	806.0455	100.8	0.8		13.7
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	13.3...	19980...		1026.3210	1026.3210	102.6	0.8		13.7
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		13.3...	447532	✓	202.3610	202.3610		0.9	✓	13.8

d Information

252.0 -> 250.0) Q1 MRMBLK-494.D



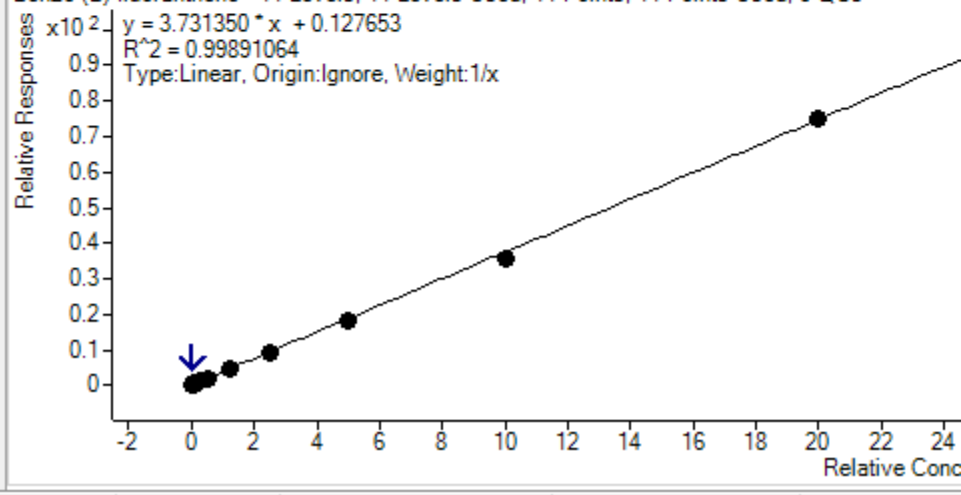
252.0 -> 250.0 , 252.0 -> 248.0



Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD

Benzo (B) fluoranthene - 11 Levels, 11 Levels Used, 11 Points, 11 Points Used, 0 QCs



Modified | 1.0 ng/ml QQQ PAH STD | Benzo (B) fluoranthene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

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Analyze Batch | Layout: | Restore Default Layout

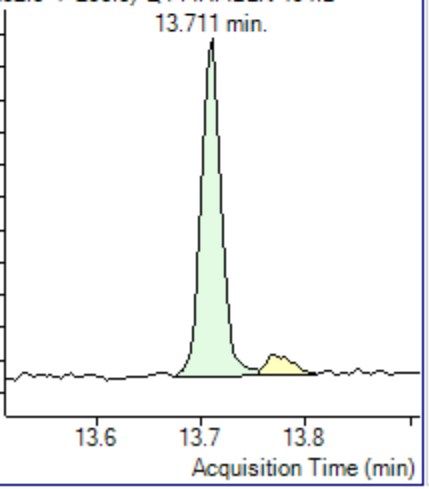
le

le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: Benzo (A) -pyrene | ISTD: Peryl

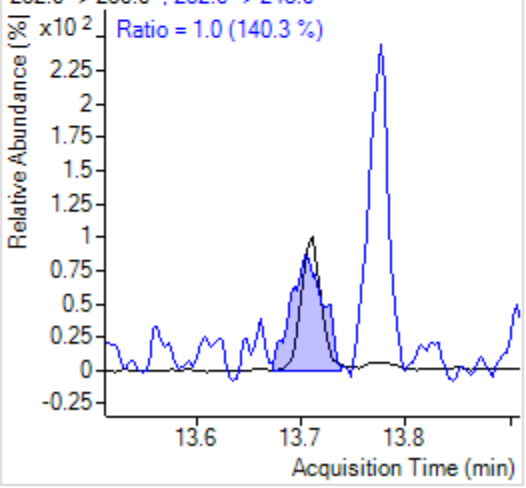
Sample					Benzo (A)...	Benzo (A) -pyrene Results					Qualifier...	Pery
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	13.7...	3489		0.8903	0.8903	89.0	1.0		13.7
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	13.7...	5225		2.3195	2.3195	116.0	0.7		13.7
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	13.7...	9345		5.0033	5.0033	125.1	0.5		13.7
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	13.7...	18831		9.9714	9.9714	99.7	0.8		13.7
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	13.7...	29105		18.1107	18.1107	90.6	0.8		13.7
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	13.7...	68401		46.2221	46.2221	92.4	0.7		13.7
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	13.7...	138377		94.5681	94.5681	94.6	0.7		13.7
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	13.7...	241927		187.9462	187.9462	94.0	0.7		13.7
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	13.7...	630441		374.8285	374.8285	93.7	0.7		13.7
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	13.7...	12809...		809.5041	809.5041	101.2	0.7		13.7
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	13.7...	15528...		1037.6359	1037.6359	103.8	0.7		13.7
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		13.7...	683145	✓	403.3437	403.3437		0.6		13.8

d Information

252.0 -> 250.0) Q1 MRMBLK-494.D



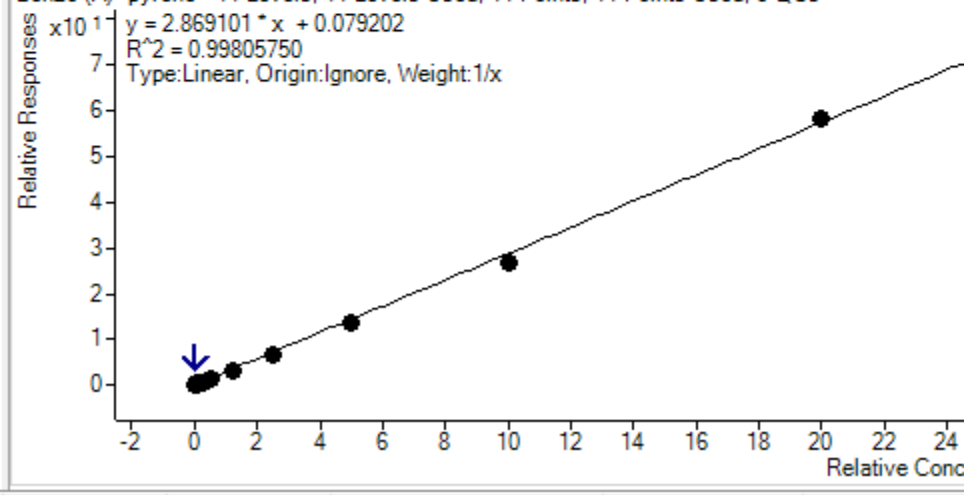
252.0 -> 250.0 , 252.0 -> 248.0



Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD

Benzo (A) -pyrene - 11 Levels, 11 Levels Used, 11 Points, 11 Points Used, 0 QCs



Modified | 1.0 ng/ml QQQ PAH STD | Benzo (A) -pyrene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

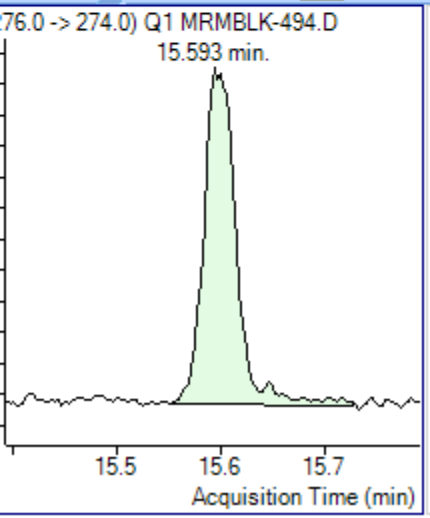
Analyze Batch | Layout: | Restore Default Layout

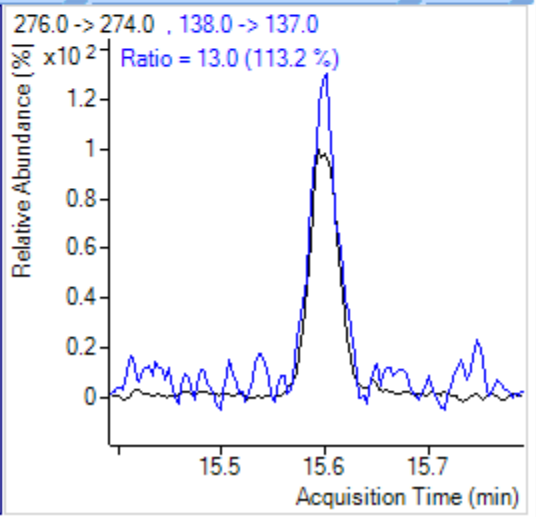
le

le: 1.0 ng/ml QQQ PAH STD | Sample Type: <All> | Compound: Benzo(ghi)perylene | ISTD: Peryl

Sample					Benzo(ghi...	Benzo(ghi)perylene Results					Qualifier...	Pery
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	15.5...	1173		0.7535	0.7535	75.4	13.0		13.7
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	15.5...	1774		2.3398	2.3398	117.0	11.0		13.7
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	15.5...	3228		5.3927	5.3927	134.8	12.1		13.7
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	15.5...	5979		9.9255	9.9255	99.3	11.8		13.7
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	15.5...	9385		18.5612	18.5612	92.8	11.9		13.7
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	15.5...	20874		45.1383	45.1383	90.3	11.5		13.7
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	15.5...	44137		96.9370	96.9370	96.9	11.4		13.7
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	15.5...	77072		192.6887	192.6887	96.3	11.3		13.7
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	15.5...	193763		370.9525	370.9525	92.7	11.6		13.7
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	15.5...	393942		802.0084	802.0084	100.3	11.5		13.7
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	15.5...	484142		1042.3024	1042.3024	104.2	11.6		13.7
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		15.6...	48167	✓	90.4951	90.4951		10.5		13.8

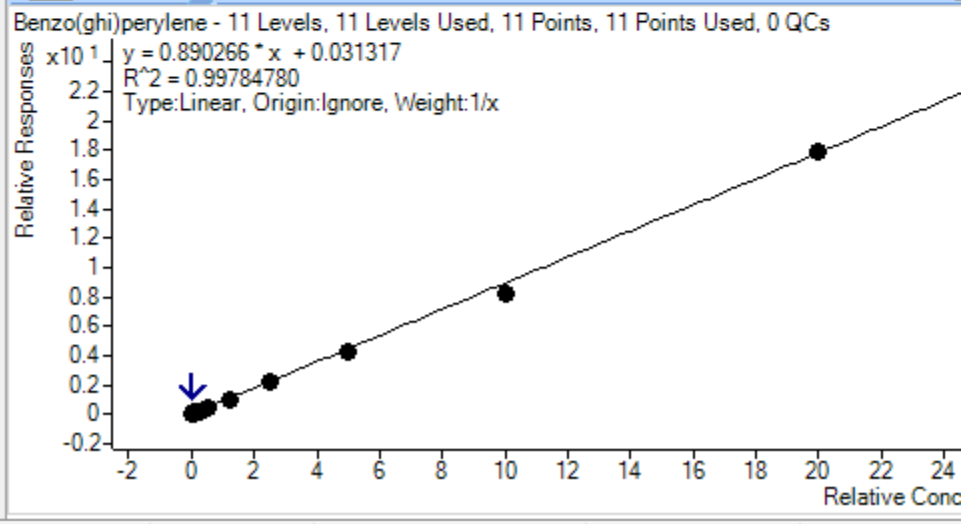
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



X 15.46 Y 116.596 | Modified | 1.0 ng/ml QQQ PAH STD | Benzo(ghi)perylene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

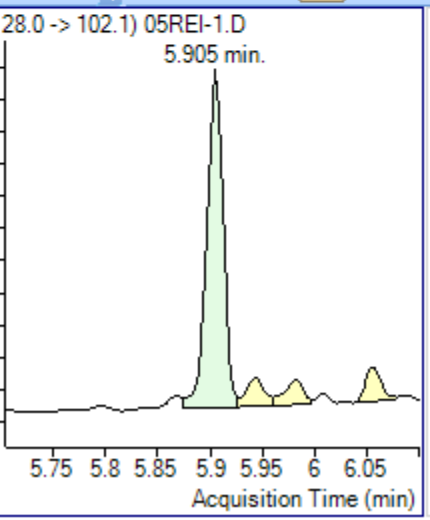
Analyze Batch | Layout: | Restore Default Layout

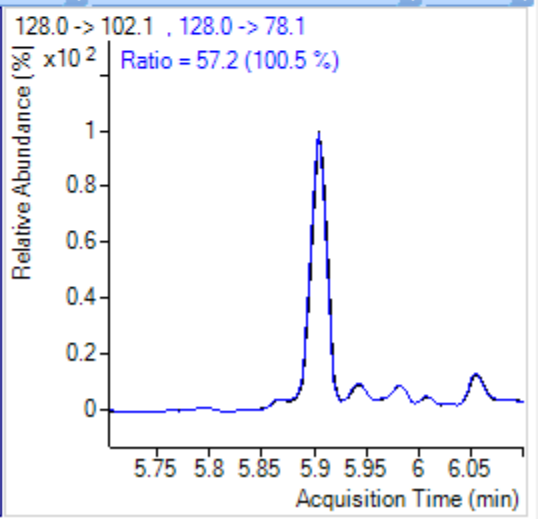
le

le: 1208012 | Sample Type: <All> | Compound: Naphthalene | ISTD: Naph

Sample					Naphthale...	Naphthalene Results					Qualifier...	Nap
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	5.905	1895		0.9506	0.9506	95.1	48.7		5.88
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	5.905	2383		2.2859	2.2859	114.3	44.4		5.88
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	5.905	3227		3.9027	3.9027	97.6	59.4		5.88
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	5.905	6625		9.6704	9.6704	96.7	56.8		5.88
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	5.905	11101		19.8132	19.8132	99.1	57.0		5.88
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	5.905	24143		49.3237	49.3237	98.6	56.9		5.88
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	5.905	49426		100.3962	100.3962	100.4	57.3		5.88
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	5.905	82991		196.4145	196.4145	98.2	56.9		5.88
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	5.905	207541		398.6132	398.6132	99.7	57.0		5.88
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	5.905	406513		793.4825	793.4825	99.2	57.2		5.88
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	5.905	493237		1012.1470	1012.1470	101.2	57.1		5.88
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		5.905	28901		51.9733	51.9733		57.2		5.88

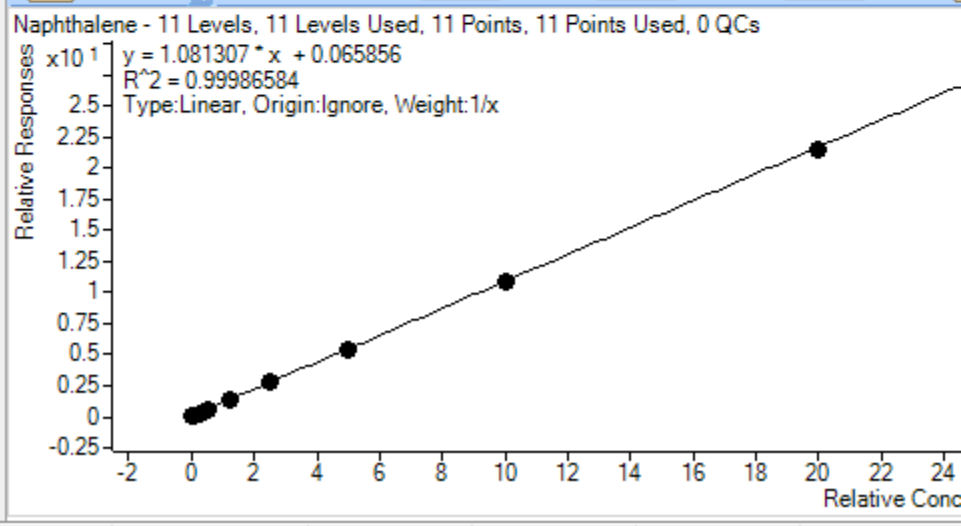
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



X 5.85 Y 105.482 | Modified | 1208012 | Naphthalene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

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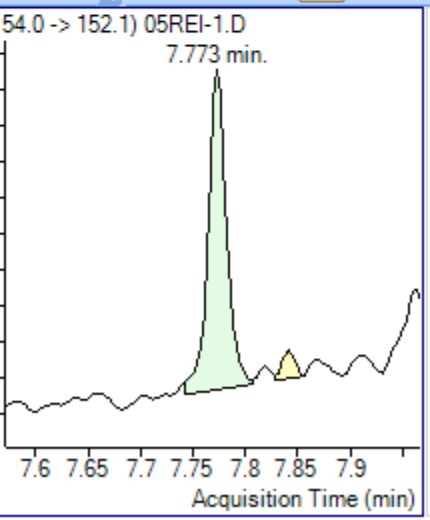
Analyze Batch | Layout: | Restore Default Layout

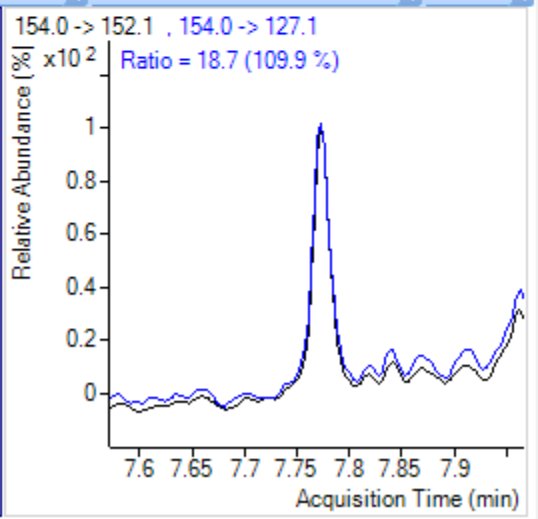
le

le: 1208012 | Sample Type: <All> | Compound: Acenaphthene | ISTD: Acen

Sample					Acenapht...	Acenaphthene Results					Qualifier...	Ace
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	7.770	1028		0.4433	0.4433	44.3	20.7		7.73
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	7.770	1756		2.3999	2.3999	120.0	18.9		7.73
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	7.770	2992		5.1296	5.1296	128.2	18.2		7.73
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	7.770	6125		11.1298	11.1298	111.3	16.9		7.73
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	7.770	9345		19.7954	19.7954	99.0	16.8		7.73
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	7.770	21102		49.7423	49.7423	99.5	17.0		7.73
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	7.770	41650		99.9773	99.9773	100.0	16.9		7.73
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	7.770	70755		196.0929	196.0929	98.0	16.9		7.73
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	7.770	177054		396.6438	396.6438	99.2	17.0		7.73
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	7.770	349751		797.1452	797.1452	99.6	17.1		7.73
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	7.770	420477		1008.5005	1008.5005	100.9	17.1		7.73
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		7.773	21696		46.0676	46.0676		18.7		7.73

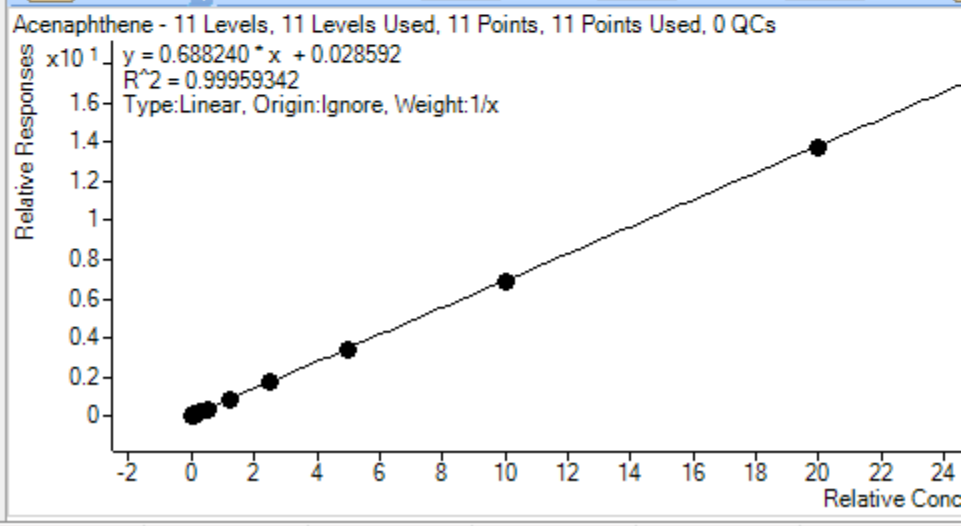
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1208012 | Acenaphthene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

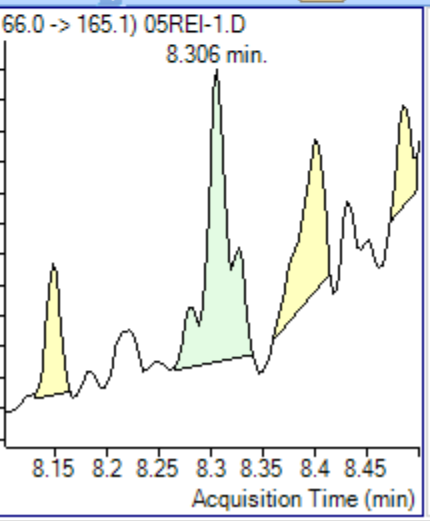
Analyze Batch | Layout: | Restore Default Layout

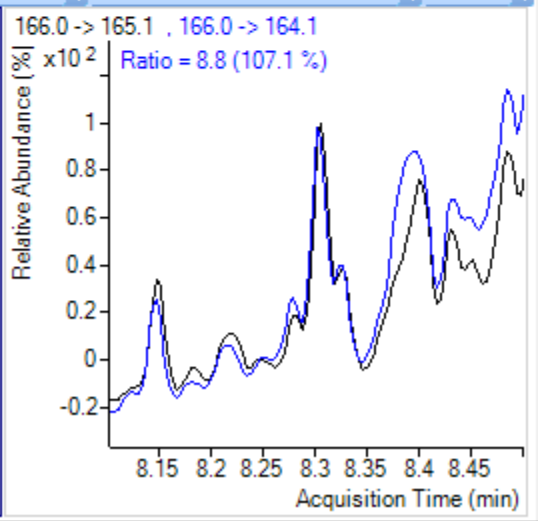
ple

le: 1208012 | Sample Type: <All> | Compound: Fluorene | ISTD: Acen

Sample					Fluorene...	Fluorene Results					Qualifier...	Acer
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	8.303	2793		0.4356	0.4356	43.6	8.1		7.73
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	8.303	4556		2.3053	2.3053	115.3	8.7		7.73
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	8.303	7933		5.2080	5.2080	130.2	8.5		7.73
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	8.303	16424		11.5352	11.5352	115.4	8.2		7.73
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	8.303	24268		19.8553	19.8553	99.3	8.1		7.73
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	8.303	54497		49.7716	49.7716	99.5	8.2		7.73
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	8.303	106995		99.6161	99.6161	99.6	8.2		7.73
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	8.303	181211		194.9111	194.9111	97.5	8.2		7.73
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	8.303	455825		396.4576	396.4576	99.1	8.2		7.73
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	8.303	900713		797.1462	797.1462	99.6	8.2		7.73
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	8.303	10841...		1009.7579	1009.7579	101.0	8.2		7.73
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		8.306	72169		59.8724	59.8724		8.8		7.73

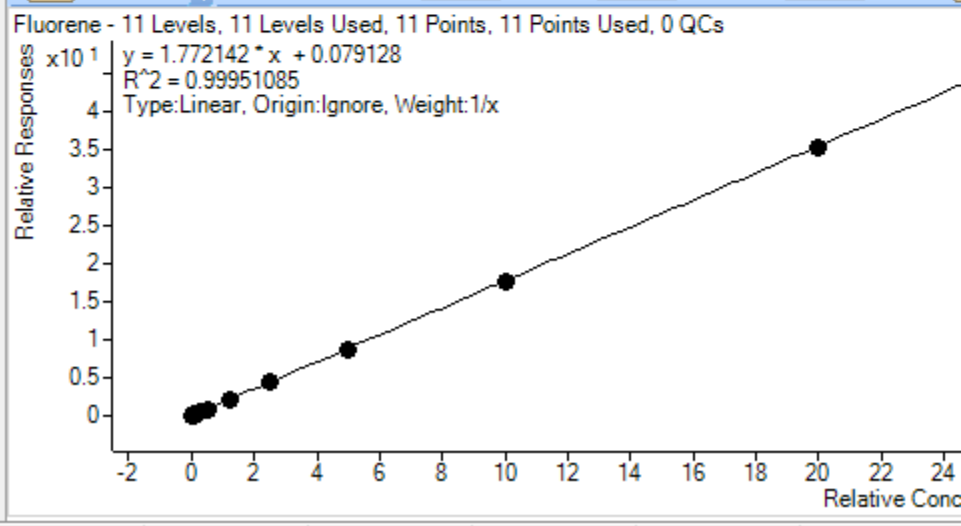
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1208012 | Fluorene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

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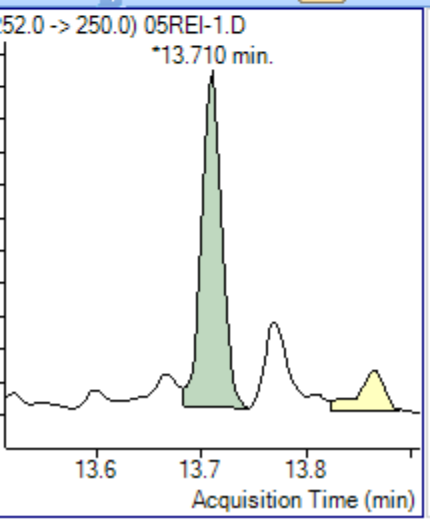
Analyze Batch | Layout: | Restore Default Layout

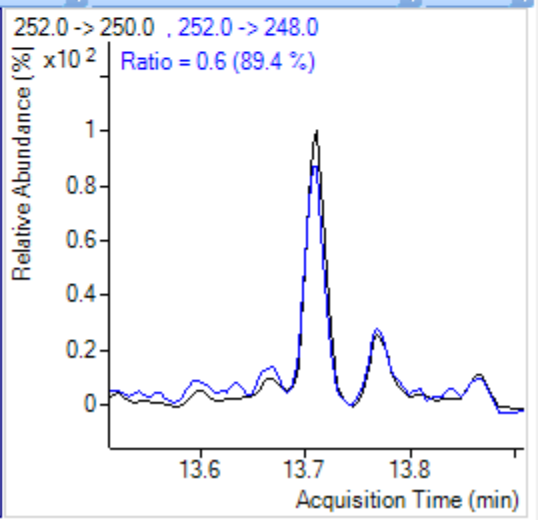
le

le: 1208012 | Sample Type: <All> | Compound: Benzo (A) -pyrene | ISTD: Peryl

Sample					Benzo (A)...	Benzo (A) -pyrene Results						Qualifier...	Pery
	Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
	1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	13.7...	3489		0.8903	0.8903	89.0	1.0		13.7
	2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	13.7...	5225		2.3195	2.3195	116.0	0.7		13.7
	4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	13.7...	9345		5.0033	5.0033	125.1	0.5		13.7
	10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	13.7...	18831		9.9714	9.9714	99.7	0.8		13.7
	20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	13.7...	29105		18.1107	18.1107	90.6	0.8		13.7
	50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	13.7...	68401		46.2221	46.2221	92.4	0.7		13.7
	100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	13.7...	138377		94.5681	94.5681	94.6	0.7		13.7
	200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	13.7...	241927		187.9462	187.9462	94.0	0.7		13.7
	400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	13.7...	630441		374.8285	374.8285	93.7	0.7		13.7
	800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	13.7...	12809...		809.5041	809.5041	101.2	0.7		13.7
	1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	13.7...	15528...		1037.6359	1037.6359	103.8	0.7		13.7
	1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		13.7...	683145	☑	403.3437	403.3437		0.6		13.8

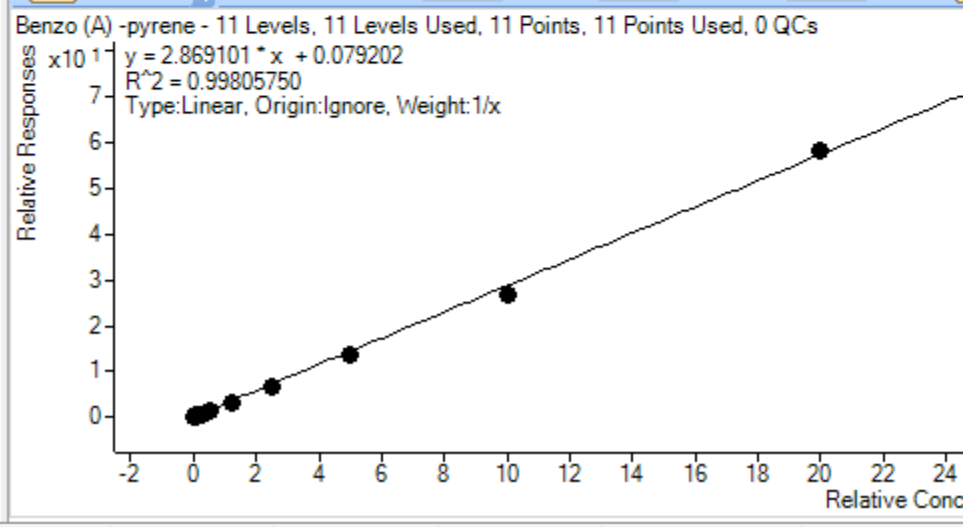
d Information





Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD



Modified | 1208012 | Benzo (A) -pyrene | 15 Samples (15

nt MassHunter Quantitative Analysis - 13_0416 - 04162013.batch.bin

dit View Analyze Method Update Report Tools Help

Analyze Batch | Layout: | Restore Default Layout

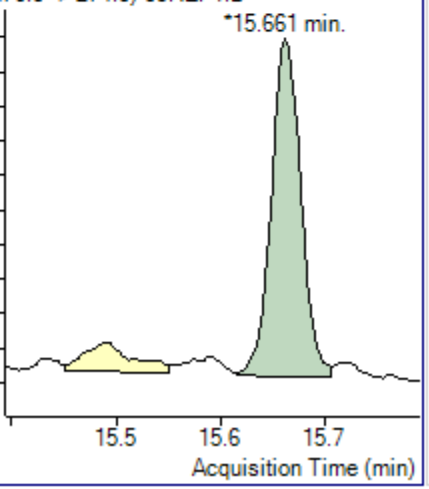
le

le: 1208012 | Sample Type: <All> | Compound: Benzo(ghi)perylene | ISTD: Peryl

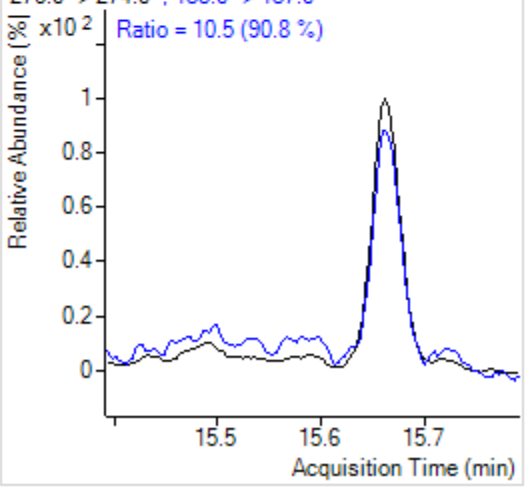
Sample					Benzo(ghi...	Benzo(ghi)perylene Results					Qualifier...	Pery
Name	Data File	Type	Level	Acq. Date-Time	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Ratio	MI	RT
1.0 ng/ml QQQ PAH STD	Q1 MRMBLK-494.D	Cal	1	4/16/2013 10:06 AM	1.0000	15.5...	1173		0.7535	0.7535	75.4	13.0		13.7
2.0 ng/ml QQQ PAH STD	Q1 MRMBLK-495.D	Cal	2	4/16/2013 10:30 AM	2.0000	15.5...	1774		2.3398	2.3398	117.0	11.0		13.7
4.0 ng/ml QQQ PAH STD	Q1 MRMBLK-496.D	Cal	3	4/16/2013 10:54 AM	4.0000	15.5...	3228		5.3927	5.3927	134.8	12.1		13.7
10 ng/ml QQQ PAH STD	Q1 MRMBLK-497.D	Cal	4	4/16/2013 11:18 AM	10.0000	15.5...	5979		9.9255	9.9255	99.3	11.8		13.7
20 ng/ml QQQ PAH STD	Q1 MRMBLK-498.D	Cal	5	4/16/2013 11:42 AM	20.0000	15.5...	9385		18.5612	18.5612	92.8	11.9		13.7
50 ng/ml QQQ PAH STD	Q1 MRMCAL-499.D	Cal	6	4/16/2013 12:07 PM	50.0000	15.5...	20874		45.1383	45.1383	90.3	11.5		13.7
100 ng/ml QQQ PAH STD	Q1 MRMCAL-500.D	Cal	7	4/16/2013 12:31 PM	100.0000	15.5...	44137		96.9370	96.9370	96.9	11.4		13.7
200 ng/ml QQQ PAH STD	Q1 MRMCAL-501.D	Cal	8	4/16/2013 12:55 PM	200.0000	15.5...	77072		192.6887	192.6887	96.3	11.3		13.7
400 ng/ml QQQ PAH STD	Q1 MRMCAL-502.D	Cal	9	4/16/2013 1:19 PM	400.0000	15.5...	193763		370.9525	370.9525	92.7	11.6		13.7
800 ng/ml QQQ PAH STD	Q1 MRMCAL-503.D	Cal	10	4/16/2013 1:43 PM	800.0000	15.5...	393942		802.0084	802.0084	100.3	11.5		13.7
1000 ng/ml QQQ PAH STD	Q1 MRMCAL-504.D	Cal	11	4/16/2013 2:08 PM	1000.0000	15.5...	484142		1042.3024	1042.3024	104.2	11.6		13.7
1208012	05REI-1.D	Sample		4/17/2013 8:00 AM		15.6...	48167	☑	90.4951	90.4951		10.5		13.8

d Information

276.0 -> 274.0) 05REI-1.D



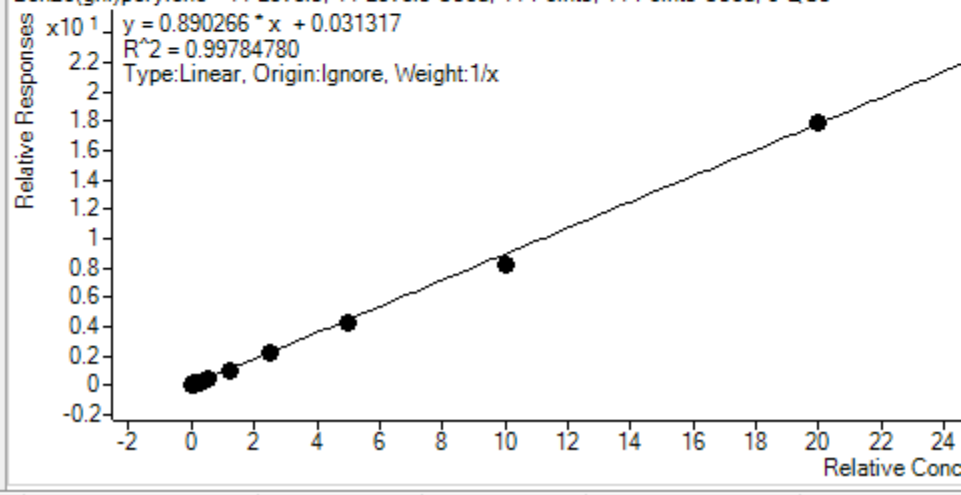
276.0 -> 274.0 , 138.0 -> 137.0



Calibration Curve

Type: Li... | Origin: I... | Weight: 1/x | ISTD

Benzo(ghi)perylene - 11 Levels, 11 Levels Used, 11 Points, 11 Points Used, 0 QCs



X 15.52 Y 27444.653 | Modified | 1208012 | Benzo(ghi)perylene | 15 Samples (15

What Labs are currently doing

- EPA Region 4 Athens, Ga
  - 8081, 8082 OC Pesticides and Arochlors
- City of Tacoma Center for Urban Waters, Wa
  - Phthalates, Arochlors, PAH's, some Phenols
  - Micro-extraction with LVI (MMI inlet)
- EPA Region 6 Houston, Tx
  - Selected 8270 analytes – PAH's etc.
- EPA Region 10 Manchester (Seattle), Wa
  - Arochlors and selected 8270 analytes
- EPA Region 8 Golden, Co
  - Expanded 8270 list (Fracking list)

Conclusions

- **GC-QQQ offers excellent sensitivity compared to ECD**
- **GC-QQQ greatly reduces interferences**
- **Toxaphene and Arochlors can be handled as summations of transitions**
- **Compound lists are easily customized with Transition Database**

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• Dale Walker	Agilent	Sacramento, Ca
• Mike Szelewski, Bruce Quimby	Agilent	Little Falls, De
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