Analysis of PAHs and PCBs in multiple matrices using GC-MS and GC-MS/MS

Andy Fornadel, PhD
Product Marketing Manager – Americas
November 15th, 2022

The world leader in serving science

Agenda

1 Introduction to polycyclic hydrocarbons

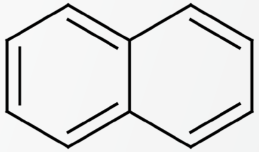
2 Challenges in GC-MS analysis using EPA method 8270E

3 Analysis of PAHs in water and soil

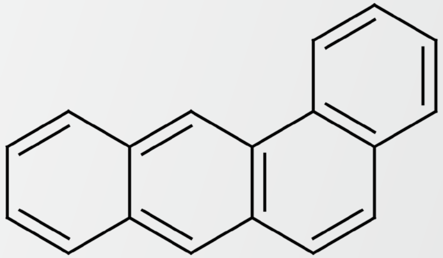
4 Conclusions

Introduction – Polycyclic Aromatic Hydrocarbons (PAHs)

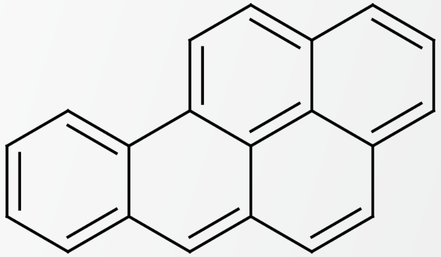
- Organic compounds consisting of 2 or more aromatic rings
- Sources:
  - Naturally occurring in fossil fuels
  - Anthropogenically produced form the incomplete combustion of organic matter (i.e., fossil fuels, wood, garbage)
- Over 100 PAH compounds identified in environmental samples



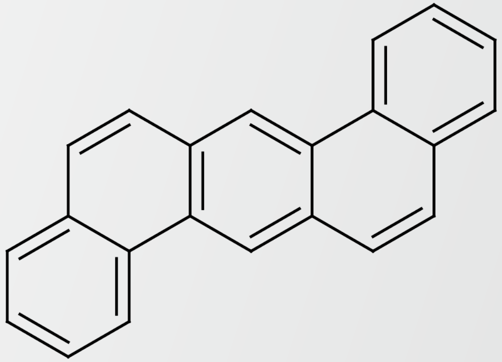
Napthalene



Benz[*a*]**anthracene**



Benzo[*a*]pyr**ene**



Dibenz[*a,h*]**anthracene**

Polycyclic Aromatic Hydrocarbons (PAHs)

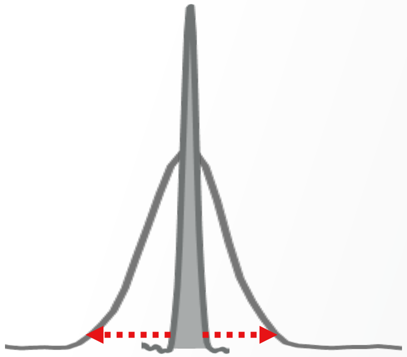
- **Wide environmental distribution**
  - Physical/Chemical properties allow for partitioning between various environmental media (air, water, soil)
- **Bioaccumulate in living organisms**
  - Exposure increases up the food chain
- **Toxic**
  - Carcinogenic
  - Genotoxicity
  - Endocrine disruptors

Gas Chromatography Mass spectrometry (GC-MS)

Semi-volatile nature of PAHs makes GC-MS an ideal tool for sample introduction and analysis

Challenges

- Sufficient chromatographic separation between PAH isomers needed to avoid isobaric interferences

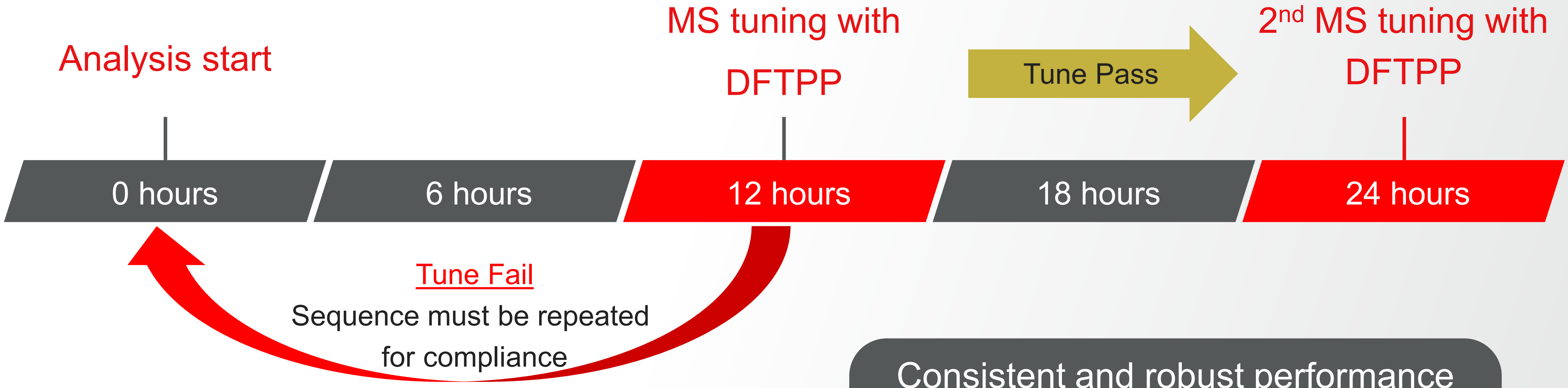


- Compounds with high boiling points prone to peak broadening and carryover between injections

- Multiple calibration curves needed to accurately quantify concentration range present in various sample matrices

Additional challenges with EPA Method 8270E

- In sequence MS tuning with 50 ng decafluorotriphenylphosphine (DFTPP) required after every 12 hours of analysis



Consistent and robust performance from GC-MS desirable for extended run times with maintenance interruptions minimized for extended up time

andy.fornadel@thermofisher.com | 15-November-2022

Analytical configuration

Thermo Fisher SCIENTIFIC

Injection parameters	
Inlet module and mode	SSL, split
Liner	P/N 453A1925-UI
Liner type and size	Thermo Scientific™ LinerGOLD™, 4 mm i.d. × 78.5 mm
Injection volume (µL)	1
Inlet temperature (˚C)	300
Split flow (mL/min)	15
Carrier gas, carrier flow (mL/min), carrier mode	He, 1.5, constant flow
Split ratio	10:1
Purge flow (mL/min)	5
Pre-injection needle wash	5 times, with DCM
Post-injection needle wash	10 times with DCM, 10 times with MeOH

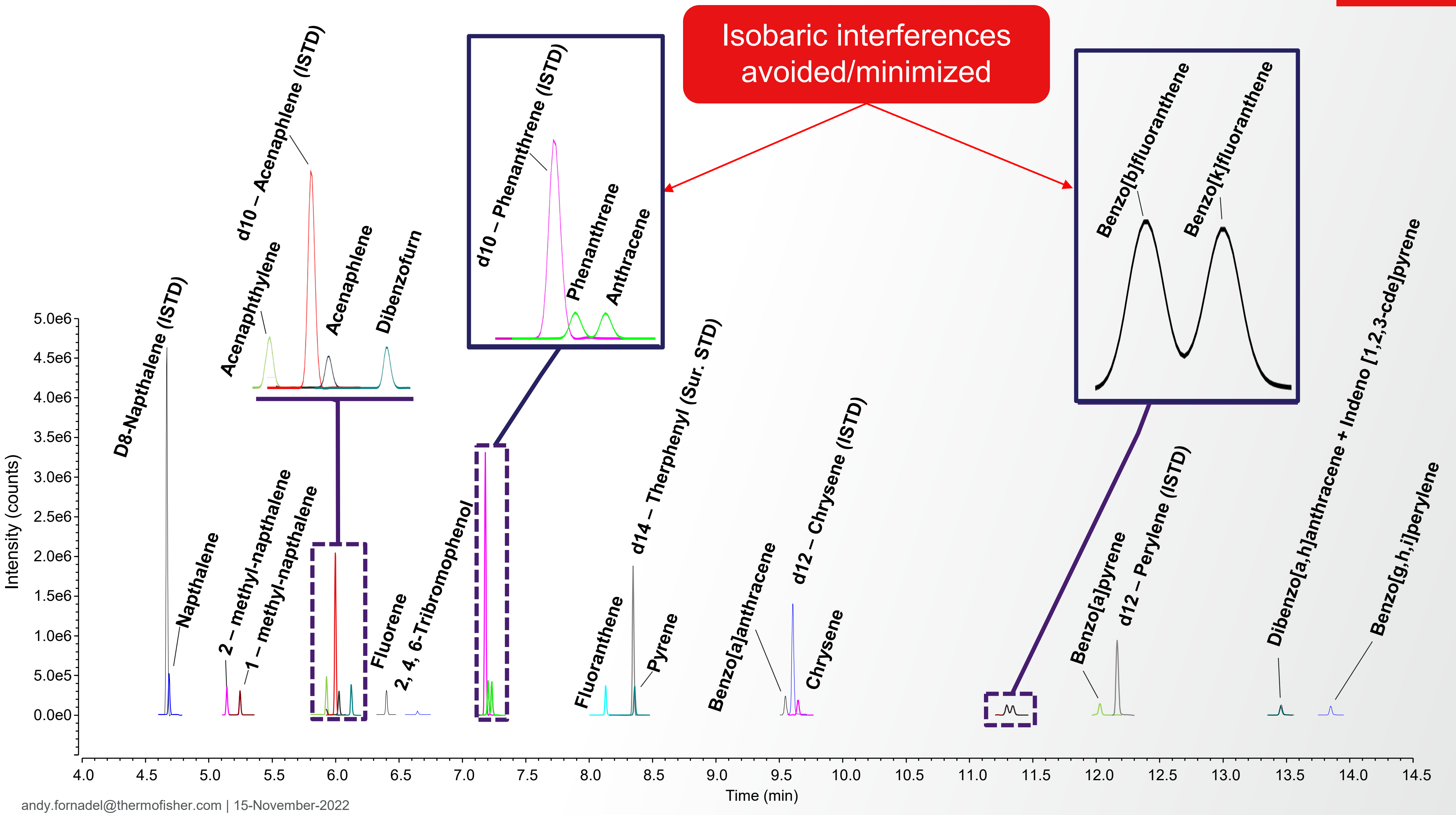
Chromatographic column	
Thermo Scientific™ TraceGOLD™ TG-PAH	P/N 26055-0470
Column dimensions	30 m × 0.25 mm i.d. × 0.10 µm

Oven temperature program	
Temperature 1 (˚C)	40
Hold time (min)	1
Temperature 2 (˚C)	285
Rate (˚C/min)	35
Temperature 3 (˚C)	295
Rate (˚C/min)	3
Temperature 4 (˚C)	350
Rate (˚C/min)	30
Hold time (min)	2
Total GC run time (min):	15.2

MS parameters	
Ion source	ExtractaBrite
Transfer line temperature (˚C)	350
Ion source temperature (˚C)	350
Ionization type	EI
Electron energy (eV)	70
Emission current (µA)	10
Acquisition mode	SIM, 2 ions/compound

Compound name	Rt (min)	MS quantifier ion (*m/z*)	MS confirmatory ion (*m/z*)
Naphthalene-d_8	4.7	136	108
Naphthalene	4.8	128	129
2 - methyl Naphthalene	5.2	142	141
1 - methyl Naphthalene	5.3	142	141
Acenaphthylene	5.9	152	151
Acenaphthene	6.0	153	154
Acenaphthene-d_{10}	6.0	162	164
Dibenzofuran	6.1	168	139
Fluorene	6.4	165	166
Phenanthrene-d_{10}	7.2	188	184
Phenanthrene	7.2	178	176
Anthracene	7.2	178	176
Fluoranthene	8.1	202	200
Terphenyl-d_{14}	8.3	244	122
Pyrene	8.4	202	200
Benz[*a*]anthracene	9.5	228	226
Chrysene-d_{12}	9.7	240	236
Chrysene	9.7	228	226
Benzo[*b*]fluoranthene	11.3	252	250
Benzo[*k*]fluoranthene	11.4	252	250
Benzo[*a*]pyrene	12.1	252	250
Perylene-d_{12}	12.2	264	260
Dibenzo[*a,h*]anthracene	13.5	278	139
Indeno[1,2,3-*cd*]pyrene	13.5	276	138
Benzo[*g,h,i*]perylene	13.9	276	138

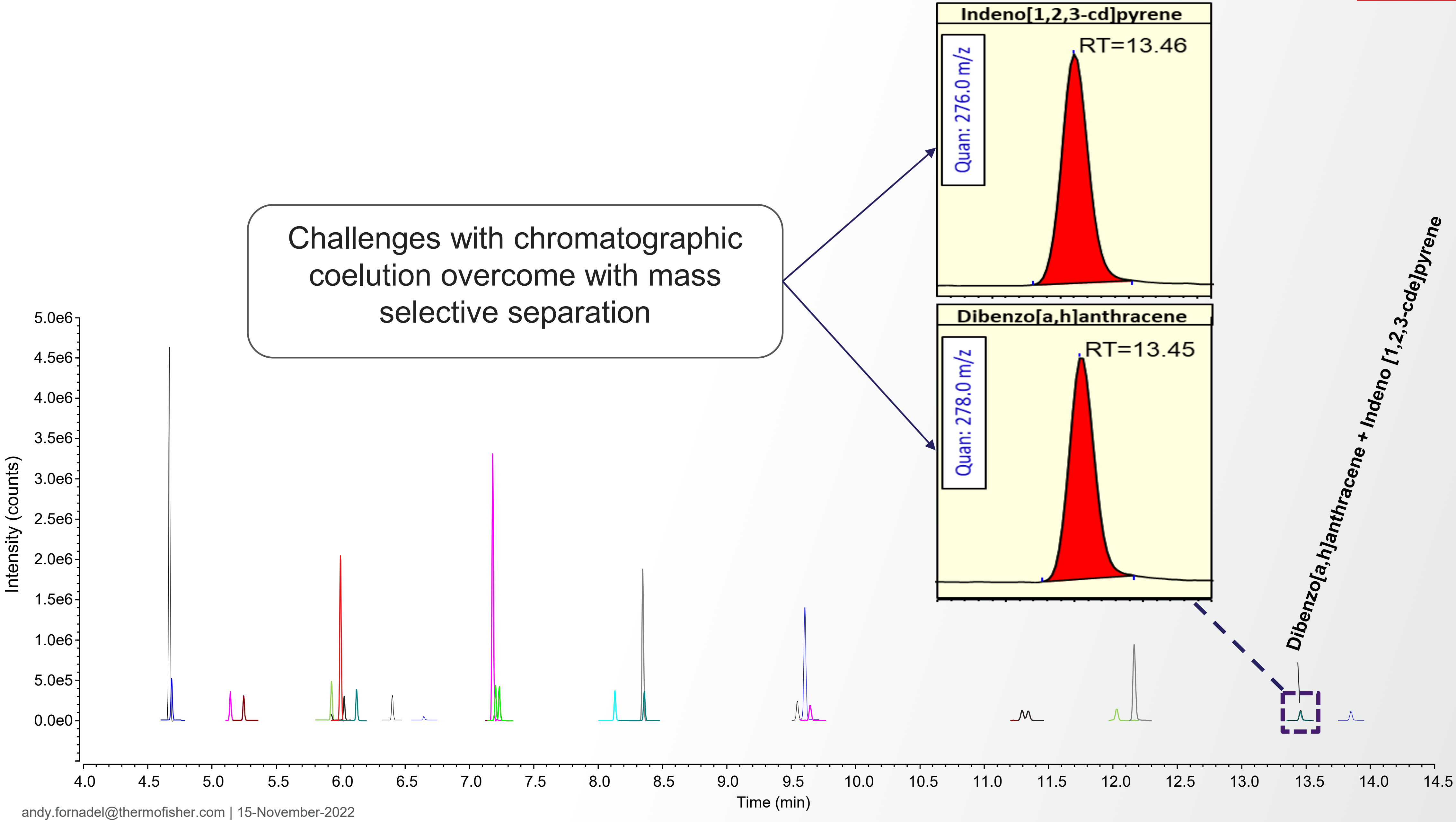
Chromatographic separation and isomer resolution



andy.fornadel@thermofisher.com | 15-November-2022

Chromatographic separation and isomer resolution

Challenges with chromatographic coelution overcome with mass selective separation



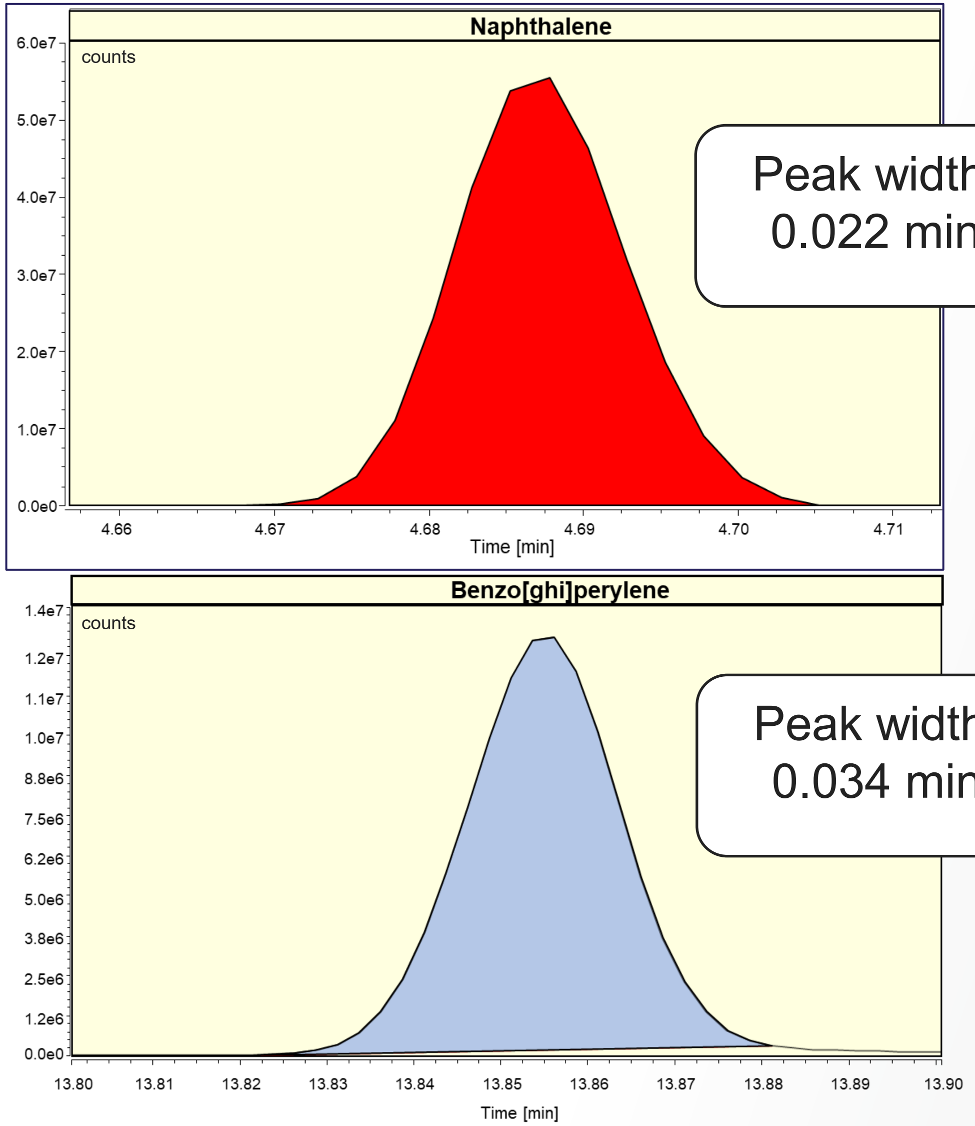
andy.fornadel@thermofisher.com | 15-November-2022

Chromatography

EPA Method 8270E criteria – Peak broadening

First eluting

Last eluting



Peak width: 0.022 min

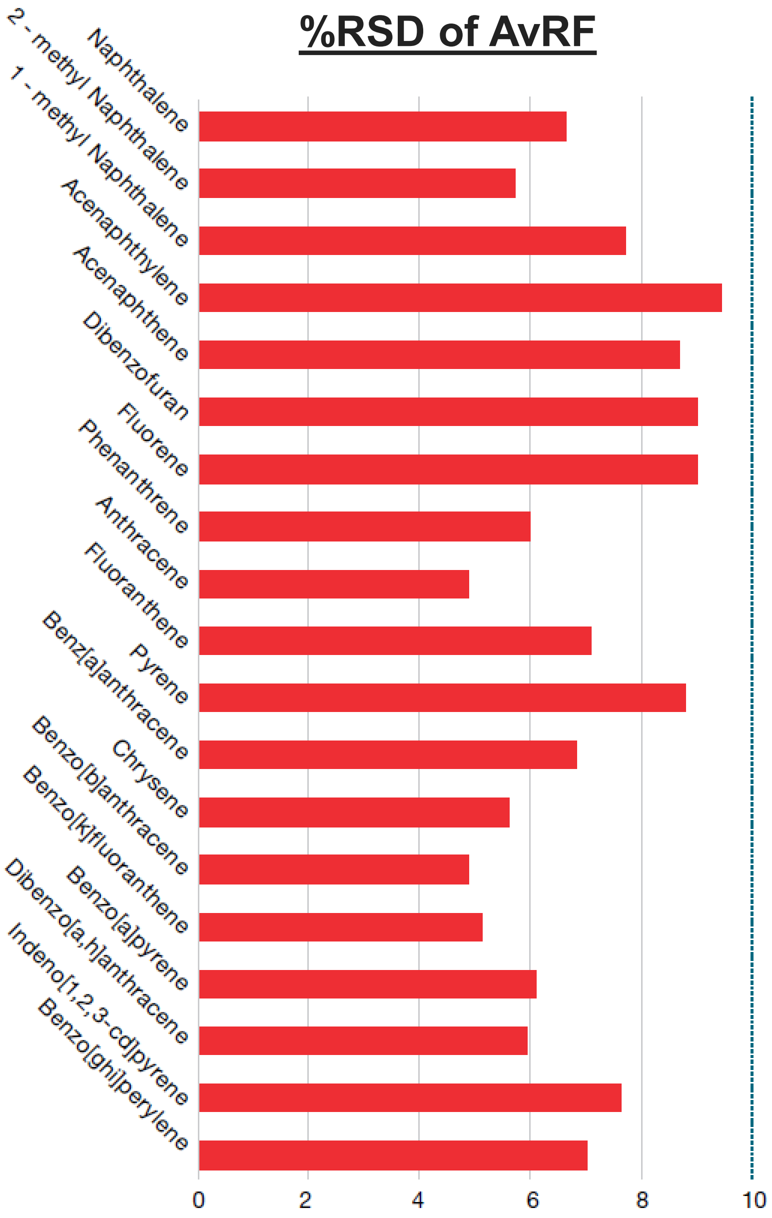
Peak width: 0.034 min

Minimal peak broadening observed between early and late eluting compounds

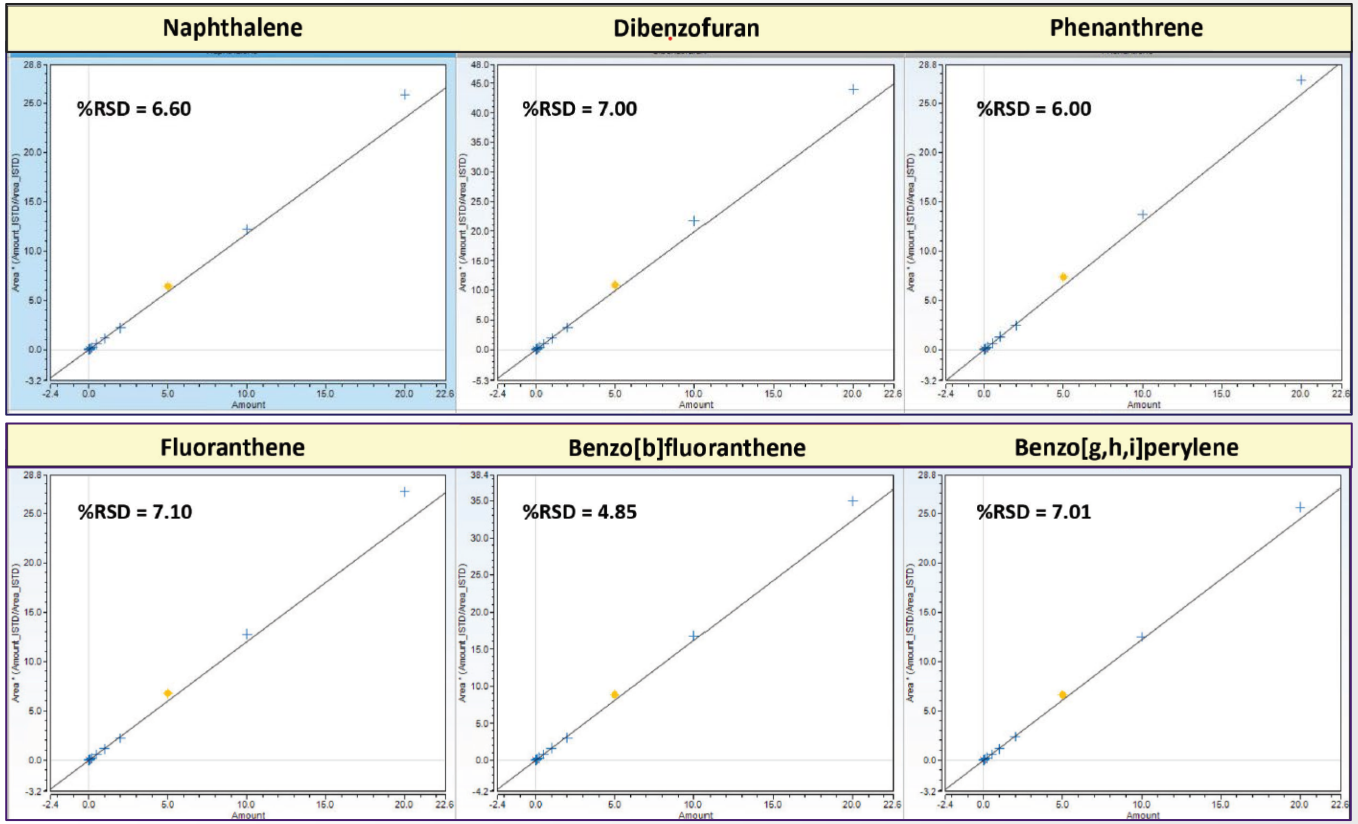
 andy.fornadel@thermofisher.com | 15-November-2022

Response linearity

%RSD of AvRF



Calibration range: 2.5 – 20,000 ng/ml



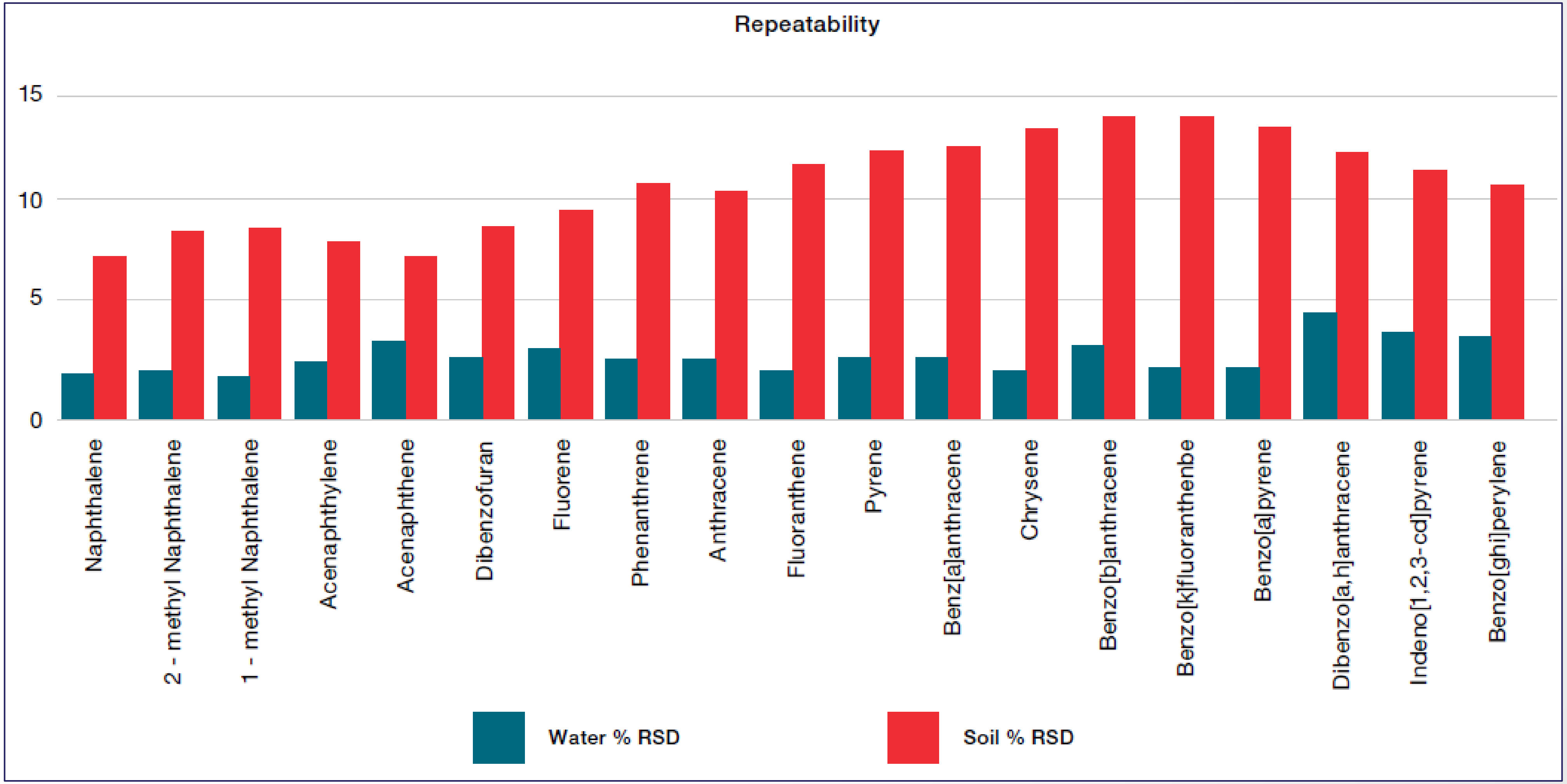
- Average relative response factor (AvRF) calibration variation below EPA Method 8270E criteria (%RSD < 15%)
- Quantitation possible at trace levels and high contamination levels with single calibration curve

Performance towards PAH analysis in water and soil

1. Repeatability in sample matrices
2. Instrument robustness using EPA method 8270E
3. In sequencing tune and calibration checks

Repeatability

- 20 ng/mL spiked in blank water and soil QC matrices (n = 10)

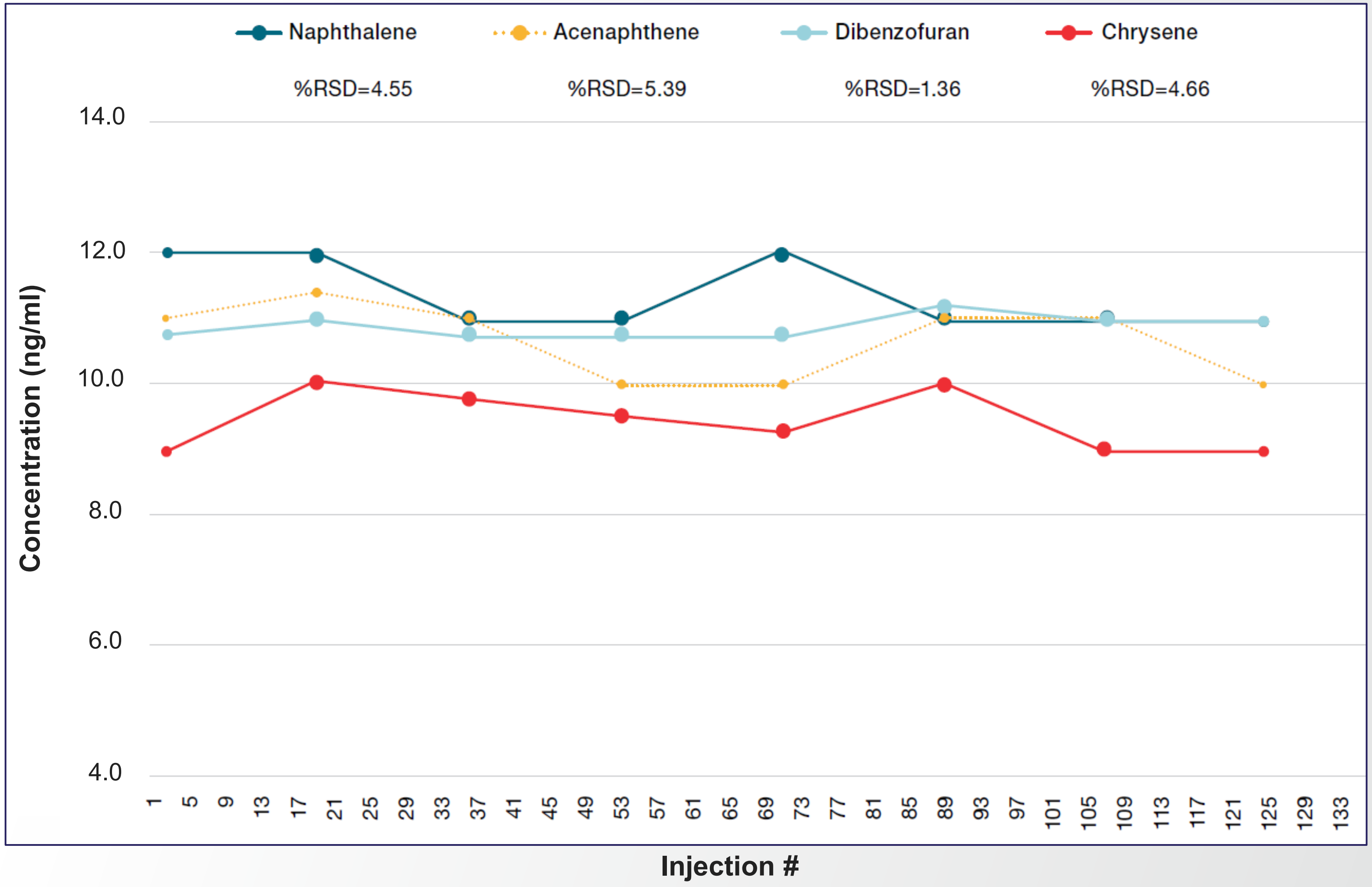


Reproducibility – Water analysis

Water QC sample at 10 ng/ml

<u>%RSD < 10% </u>after 133 consecutive injections (52 hours) without any GC or MS maintenance:

- Liner change
- Column trimming
- MS cleaning

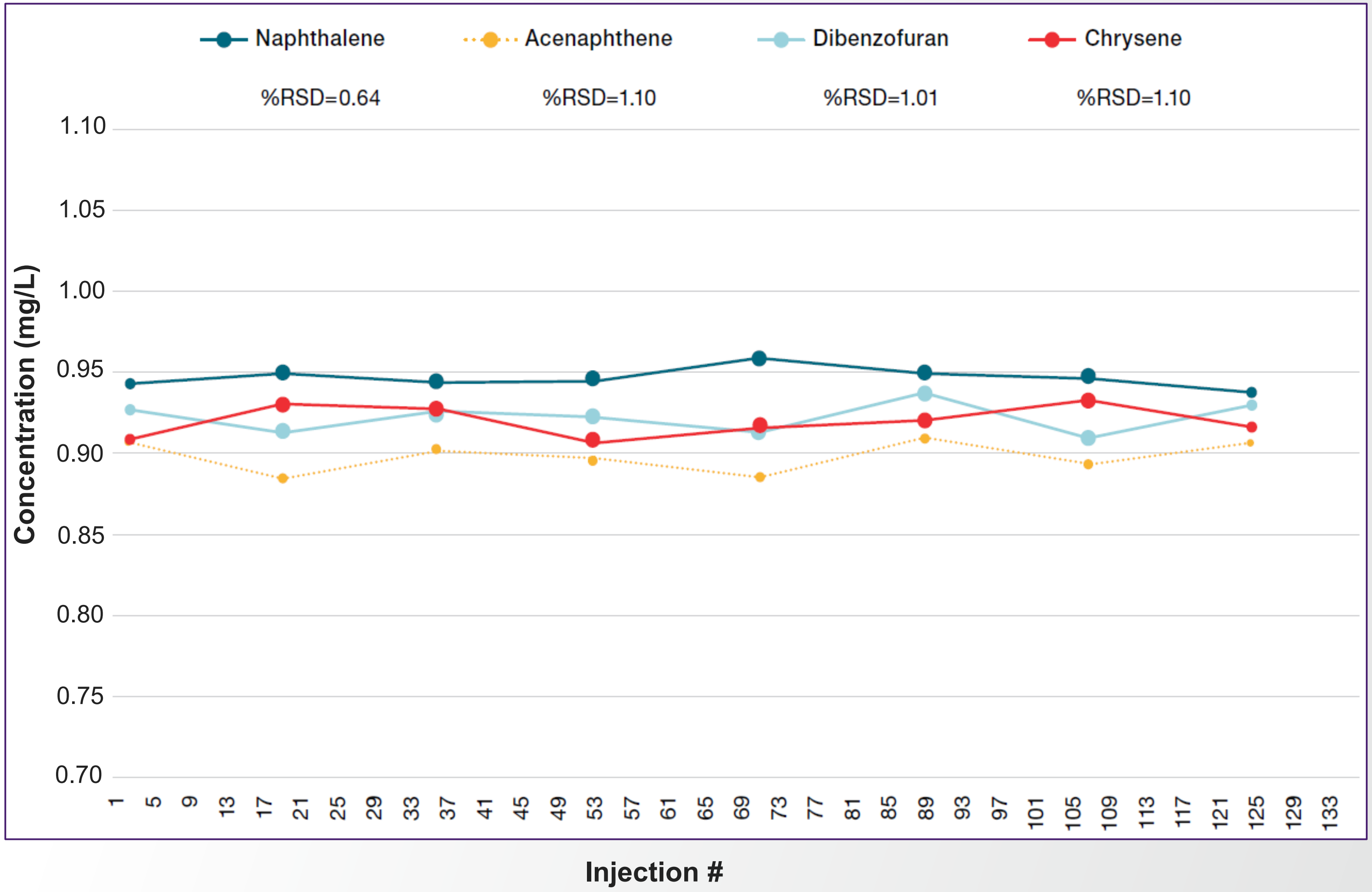


Reproducibility – Soil analysis

Soil QC sample at 1.0 mg/L

<u>%RSD < 10%</u> after 133 consecutive injections (52 hours) without any GC or MS maintenance:

- Liner change
- Column trimming
- MS cleaning

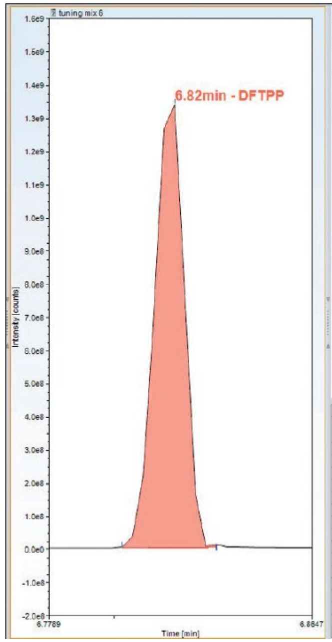


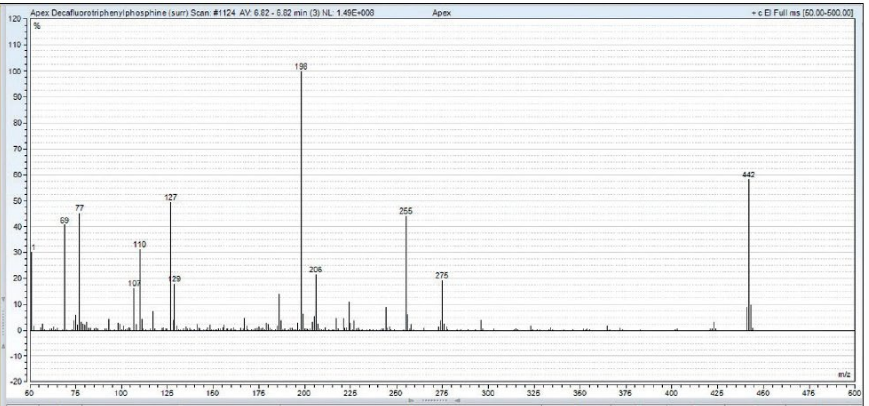
 andy.fornadel@thermofisher.com | 15-November-2022

In sequence tuning, calibration and QC checks

ThermoFisher SCIENTIFIC

MS tuning verification every 6 hours with DFTPP in full scan with report automatically generated





	A	B	C	D	E	F	G	H
1	Number	Name	Tested Injections	Test Result	Eval. Result	Operator	Ref. Value (1)	Ref. Value (2)
2	1	m/z 51 - 10 to 80% of the base peak	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	30	between	10	80
3	2	m/z 68 - Less than 2% of m/z 69	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	0	<	2	
4	3	m/z 70 - Less than 2% of m/z 69	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	0	<	2	
5	4	m/z 127 - 10 to 80% of the base peak	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	49	between	10	80
6	5	m/z 197 - Less than 2% of m/z 198	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	0	<	2	
7	6	m/z 198 - Greater than 50% of m/z 442	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	172	>	50	
8	7	m/z 199 - 5 to 9% of m/z 198	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	6	between	5	9
9	8	m/z 275 - 10 to 60% of the base peak	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	19	between	10	60
10	9	m/z 365 - Greater than 1% of m/z 198	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	2	>	1	
11	10	m/z 441 - Present	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	13,406,901	>	0	
12	11	m/z 441 - Less than 24% of m/z 442	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	16	<	24	
13	12	m/z 442 - Greater than 50% of m/z 198	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	58	>	50	
14	13	m/z 443 - 15 to 24% of m/z 442	(injection.customVar("Analysis_Type")="MS Tune Check")	Passed	17	between	15	24
15		Number of executed test cases:	13	Passed				
16								

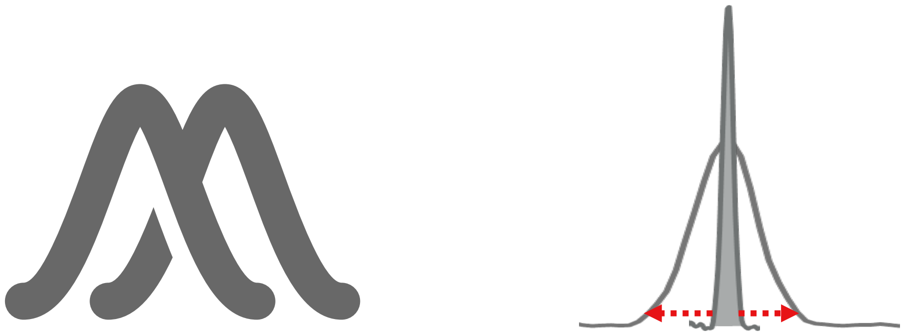
Summary View / Peak Results / Library Search / System Suitability Tests / Calibration / Audit Trail

#	TIC	Name	Type	Position	Instrument Method	Status	Analysis_Type
1		DCM	Unknown	54	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
2		tuning mix 1	Unknown	53	PAHs SIM - 10uA - SPLIT 10to1 - FS	Finished	Field Sample
3		QC low water	Unknown	1	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
4		QC low soil	Unknown	2	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
5		QC middle water	Unknown	3	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
6		QC middle soil	Unknown	4	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
7		QC high water	Unknown	5	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
8		QC high soil	Unknown	6	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
9		Cali check 0.0025	Unknown	10	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
10		s1	Unknown	55	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
11		s2	Unknown	56	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
12		s3	Unknown	57	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
13		s4	Unknown	58	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
14		s5	Unknown	59	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
15		s6	Unknown	60	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
16		s7	Unknown	61	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
17		s8	Unknown	62	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
18		s9	Unknown	63	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
19		tuning mix 2	Unknown	53	PAHs SIM - 10uA - SPLIT 10to1 - FS	Finished	Field Sample
20		Cali check 0.005	Unknown	11	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
21		QC low water 2	Unknown	1	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
22		QC low soil 2	Unknown	2	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
23		QC middle water 2	Unknown	3	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
24		QC middle soil 2	Unknown	4	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
25		QC high water 2	Unknown	5	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
26		QC high soil 2	Unknown	6	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
27		s10	Unknown	64	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample
28		s11	Unknown	65	PAHs SIM - 10uA - SPLIT 10to1	Finished	Field Sample

Routine calibration and sample QC checks at different concentrations to ensure analysis accuracy

- Calibration accuracy: ± 10%
- Spiked recovery: 80 – 120 %

Conclusions - PAHs



Efficient chromatographic separation within 14.5 min with minimal peak broadening by late eluting compounds and isobaric interferences avoided

Linear dynamic range over 4 orders of magnitude allowing multiple sample types to be analyzed on a single calibration curve.

Robust analysis of PAHs was demonstrated with %RSD < 10% for sample QCs after 133 consecutive injections with no GC or MS maintenance

Spike recoveries of sample QC range from 80-120% with method detection limits ranging from 0.5 – 7.6 pg on column

In sequence tuning and report generation automatically provides compliance requirements for EPA method 8270E and allowing for maximum instrument up time

andy.fornadel@thermofisher.com | 15-November-2022

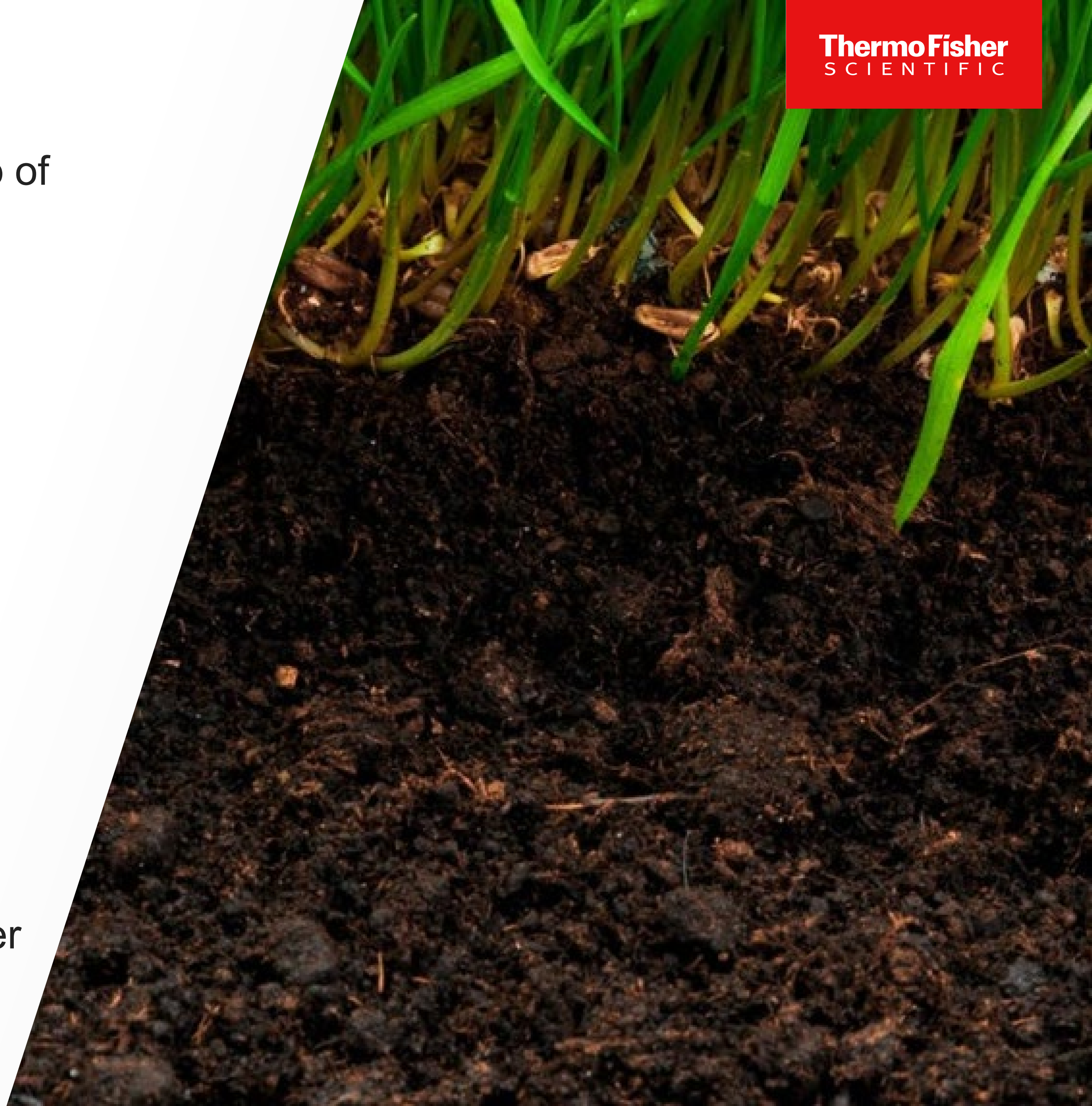
Content

Introduction

Polychlorinated biphenyls (PCBs) are a group of industrial organic chemicals characterized by:

- non-flammability
- chemical stability
- high boiling point
- electrical insulating properties
- persistence in environment

Many of these properties make PCBs historically useful in electrical insulators, hydraulic equipment, paints, rubbers, and other industrial applications



PCB congeners

Currently 209 known PCBs congeners that can be divided into two groups according to their structural and toxicological characteristics:

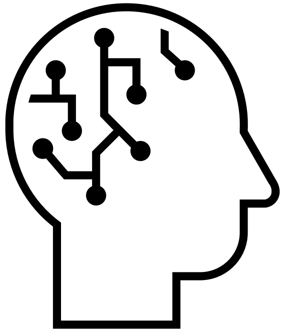
- non-dioxin like PCBs (non-DL-PCB):
  - majority of the PCB congeners
  - lower degree of toxicity
- dioxin-like PCBs (DL-PCBs):
  - the 12 most toxic congeners
  - classified as POPs
  - regulated under the Stockholm Convention for POPs since 2001

GC-MS/MS for analysis of PCBs

- EPA developed Method 1668 using GC-HRMS
- Advances in GC-MS/MS allows for reliable application to PCB analysis.
  - Different extraction and clean-up processes
  - More sensitive/selective mass analyzers and column phases
  - Re-evaluation of performance metrics
- Important parameters to consider:
  - Working range, particularly on the low-end
  - Linearity, reproducibility, robustness
  - Applicability for routine analysis.

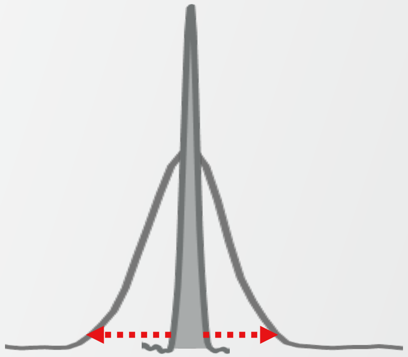
Traditional challenges

Challenges



- Complicated sample preparation

- Sufficient chromatographic separation between PCBs needed to avoid isobaric interferences



- Long run times for sufficient separations. Low throughput and high costs.

andy.fornadel@thermofisher.com | 15-November-2022

Analytical parameters

AI/AS 1610 autosampler parameters	
Injection type	Standard
Sample mode	Standard
Fill strokes	10
Sample depth	Bottom
Injection mode	Fast
Pre-injection delay time (s)	0
Post-injection delay time (s)	0
Pre-injection wash cycles	0
Post-injection wash cycles	4
Post-injection solvent wash volume (µL)	6.0
Sample wash cycles	1
Sample wash volume (µL)	1.0
Injection volume (µL)	1.0

SSL parameters	
Injection temperature (°C)	280
Liner	Thermo Scientifc™ LinerGOLD™ splitless/split liner single taper with wool (P/N 453A1925-UI)
Inlet module and mode	SSL, splitless
Split flow (mL/min)	75
Splitless time (min)	1.2
Septum purge flow (mL/min)	5, constant
Carrier gas, flow (mL/min)	He, 1.2

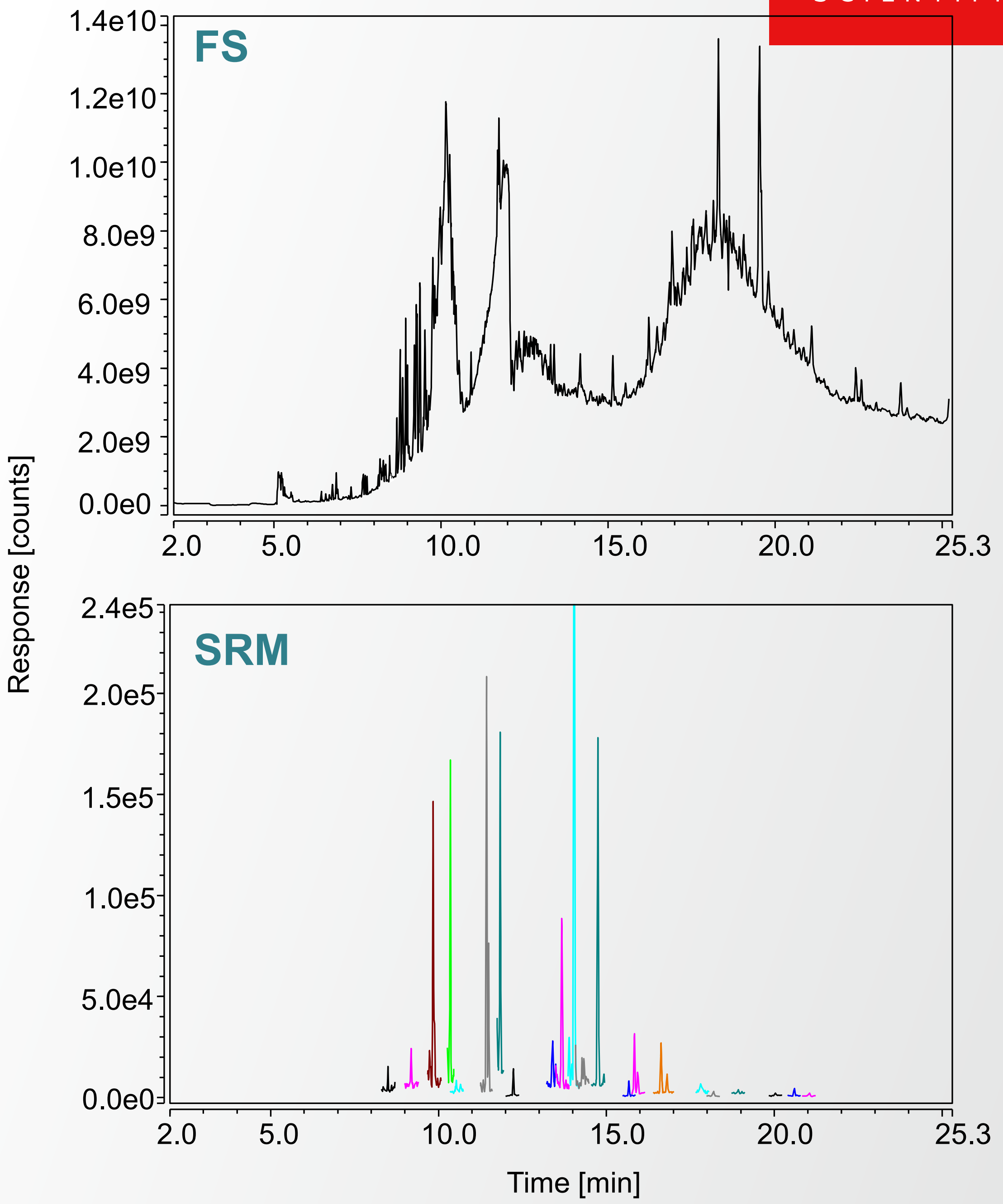
TRACE 1610 GC parameters	
Oven temperature program	
Temperature (°C)	90
Hold time (min)	1.00
Rate (°C/min)	25
Temperature 2 (°C)	270
Rate 2 (°C/min)	4
Temperature 3 (°C)	330
Hold time (min)	2
GC run time (min)	25.20
Column	
TRACE TR-PCB 8 MS	50 m, 0.25 mm, 0.25 µm (P/N 26AJ148P)

TSQ 9610 mass spectrometer parameters	
Transfer line temperature (°C)	280
Ion source type and temperature (°C)	NeverVent AEI, 300
Ionization type	EI
Emission current (µA)	50
Aquisition mode	timed-SRM
Q1 and Q3 resolution	Normal (0.7 amu)
Tuning parameters	AEI SmartTune
Collision gas and pressure (psi)	Argon at 70
Detector gain	X 7

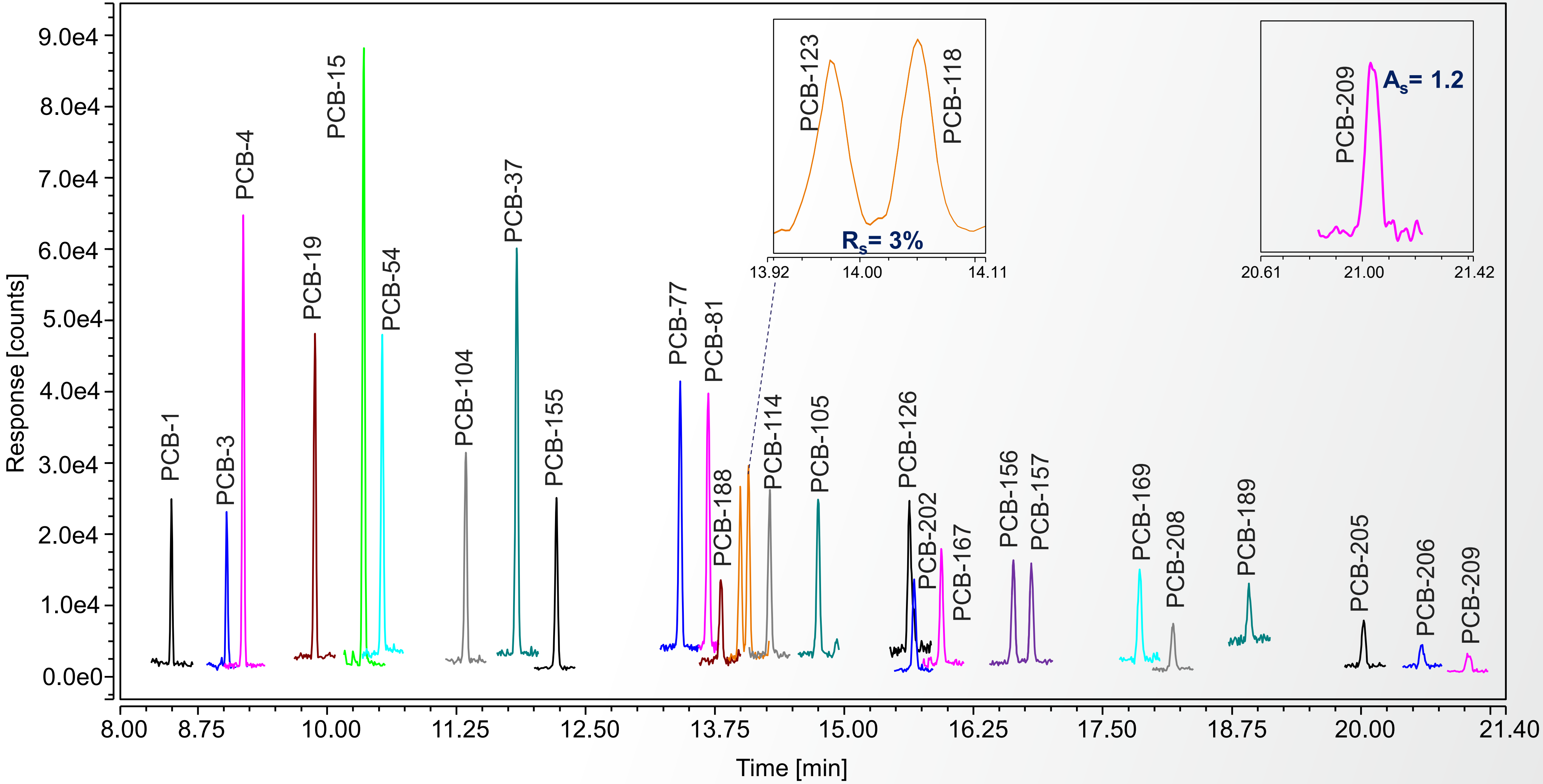
t-SRM for improved selectivity

Compound	Retention time (min)	Precursor Ion (Da)	Product Ion (Da)	Collision Energy (V)
PCB-1	8.5	188.04	153.04	22
PCB-1	8.5	190.04	153.04	22
PCB-1L13C	8.5	200.08	165.10	22
PCB-1L13C	8.5	202.08	165.10	22
PCB-3	9.03	188.04	153.04	22
PCB-3	9.03	190.04	153.04	22
PCB-3L13C	9.03	200.08	165.10	22
PCB-3L13C	9.03	202.08	165.10	22
PCB-4	9.19	222.00	152.06	22
PCB-4	9.19	224.00	152.06	22
PCB-4L13C	9.19	234.04	164.10	22
PCB-4L13C	9.19	236.04	164.10	22
PCB-19	9.88	255.96	186.02	22
PCB-19	9.88	257.96	186.02	22
PCB-19L13C	9.88	268.00	198.02	22
PCB-19L13C	9.88	270.00	198.02	22
PCB-15	10.36	222.00	152.06	22
PCB-15	10.36	224.00	152.06	22
PCB-15L13C	10.36	234.04	164.10	22
PCB-15L13C	10.36	236.04	164.10	22
PCB-54	10.54	289.92	219.98	22
PCB-54	10.54	291.92	219.98	22
PCB-54L13C	10.54	301.96	232.02	22
PCB-54L13C	10.54	303.96	232.02	22
PCB-104	11.34	323.90	253.95	22
PCB-104	11.34	325.90	255.95	22
PCB-104L13C	11.34	335.92	265.99	22
PCB-104L13C	11.34	337.92	267.99	22
PCB-37	11.84	255.96	186.02	22
PCB-37	11.84	257.96	186.02	22
PCB-37L13C	11.84	268.00	198.02	22
PCB-37L13C	11.84	270.00	198.02	22
PCB-155	12.2	357.80	287.90	24
PCB-155	12.2	359.80	289.95	24
PCB-155L13C	12.2	369.90	299.51	24
PCB-155L13C	12.2	371.90	301.95	24
PCB-101L13C	12.59	335.92	265.99	22
PCB-101L13C	12.59	337.92	267.99	22
PCB-111L13C	13.13	335.92	265.99	22
PCB-111L13C	13.13	337.92	267.99	22
PCB-77	13.42	289.92	219.98	22
PCB-77	13.42	291.92	219.98	22
PCB-77L13C	13.42	301.96	232.02	22
PCB-77L13C	13.42	303.96	232.02	22
PCB-81	13.69	289.92	219.98	22
PCB-81	13.69	291.92	219.98	22
PCB-81L13C	13.69	301.96	232.02	22
PCB-81L13C	13.69	303.96	232.02	22
PCB-188	13.8	391.80	321.90	25
PCB-188	13.8	393.80	323.90	25
PCB-188L13C	13.8	403.80	333.90	25
PCB-188L13C	13.8	405.80	335.90	25
PCB-123	13.97	323.90	253.95	22
PCB-123	13.97	325.90	255.95	22
PCB-123L13C	13.97	335.92	265.99	22
PCB-123L13C	13.97	337.92	267.99	22

Compound	Retention time (min)	Precursor Ion (Da)	Product Ion (Da)	Collision Energy (V)
PCB-118	14.05	323.90	253.95	22
PCB-118	14.05	325.90	255.95	22
PCB-118L13C	14.05	335.92	265.99	22
PCB-118L13C	14.05	337.92	267.99	22
PCB-114	14.28	323.90	253.95	22
PCB-114	14.28	325.90	255.95	22
PCB-114L13C	14.28	335.92	265.99	22
PCB-114L13C	14.28	337.92	267.99	22
PCB-105	14.75	323.90	253.95	22
PCB-105	14.75	325.90	255.95	22
PCB-105L13C	14.75	335.92	265.99	22
PCB-105L13C	14.75	337.92	267.99	22
PCB-126	15.64	323.90	253.95	22
PCB-126	15.64	325.90	255.95	22
PCB-126L13C	15.64	335.92	265.99	22
PCB-126L13C	15.64	337.92	267.99	22
PCB-202	15.68	427.80	357.80	25
PCB-202	15.68	429.80	357.80	25
PCB-202L13C	15.68	439.80	369.90	25
PCB-202L13C	15.68	441.80	369.90	25
PCB-167	16	357.80	287.90	24
PCB-167	16	359.80	289.95	24
PCB-167L13C	16	369.90	299.51	24
PCB-167L13C	16	371.90	301.95	24
PCB-156	16.6	357.80	287.90	24
PCB-156	16.6	359.80	289.95	24
PCB-156L13C	16.6	369.90	299.51	24
PCB-156L13C	16.6	371.90	301.95	24
PCB-157	16.82	357.80	287.90	24
PCB-157	16.82	359.80	289.95	24
PCB-157L13C	16.82	369.90	299.51	24
PCB-157L13C	16.82	371.90	301.95	24
PCB-169	17.86	357.80	287.90	24
PCB-169	17.86	359.80	289.95	24
PCB-169L13C	17.86	369.90	299.51	24
PCB-169L13C	17.86	371.90	301.95	24
PCB-208	18.18	461.70	391.80	25
PCB-208	18.18	463.70	393.80	25
PCB-208L13C	18.18	473.80	403.80	25
PCB-208L13C	18.18	475.80	405.80	25
PCB-189	18.92	391.80	321.90	25
PCB-189	18.92	393.80	323.90	25
PCB-189L13C	18.92	403.80	333.90	25
PCB-189L13C	18.92	405.80	335.90	25
PCB-205	20.04	427.80	357.80	25
PCB-205	20.04	429.80	357.80	25
PCB-205L13C	20.04	439.80	369.90	25
PCB-205L13C	20.04	441.80	369.90	25
PCB-206	20.6	461.70	391.80	25
PCB-206	20.6	463.70	393.80	25
PCB-206L13C	20.6	473.80	403.80	25
PCB-206L13C	20.6	475.80	405.80	25
PCB-209	21.03	495.70	425.80	25
PCB-209	21.03	497.70	427.80	25
PCB-209L13C	21.03	507.70	437.80	25
PCB-209L13C	21.03	509.70	439.80	25



Chromatographic resolution of critical pairs

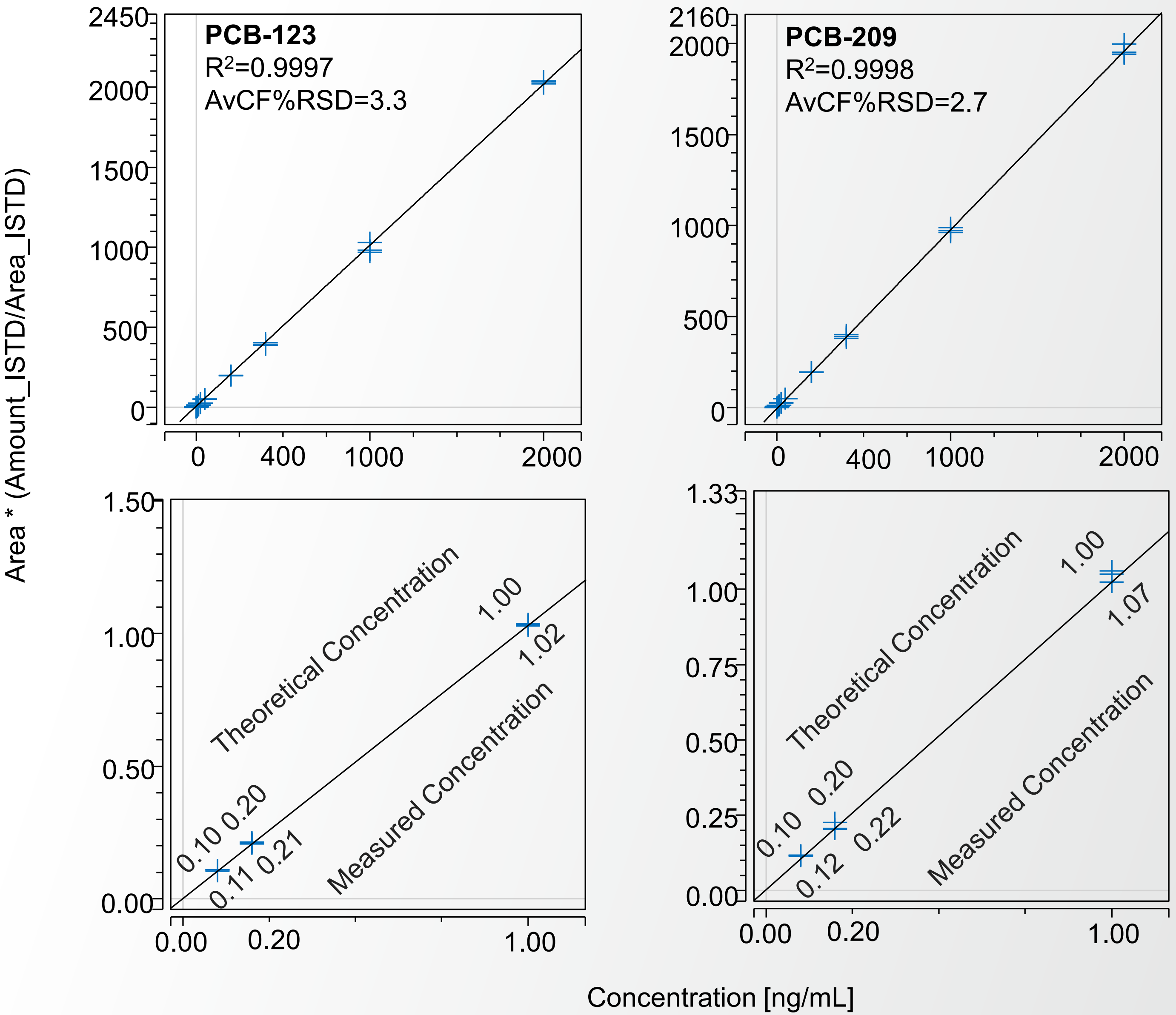


andy.fornadel@thermofisher.com | 15-November-2022

Linearity for accurate quantitative analyis

ThermoFisher SCIENTIFIC

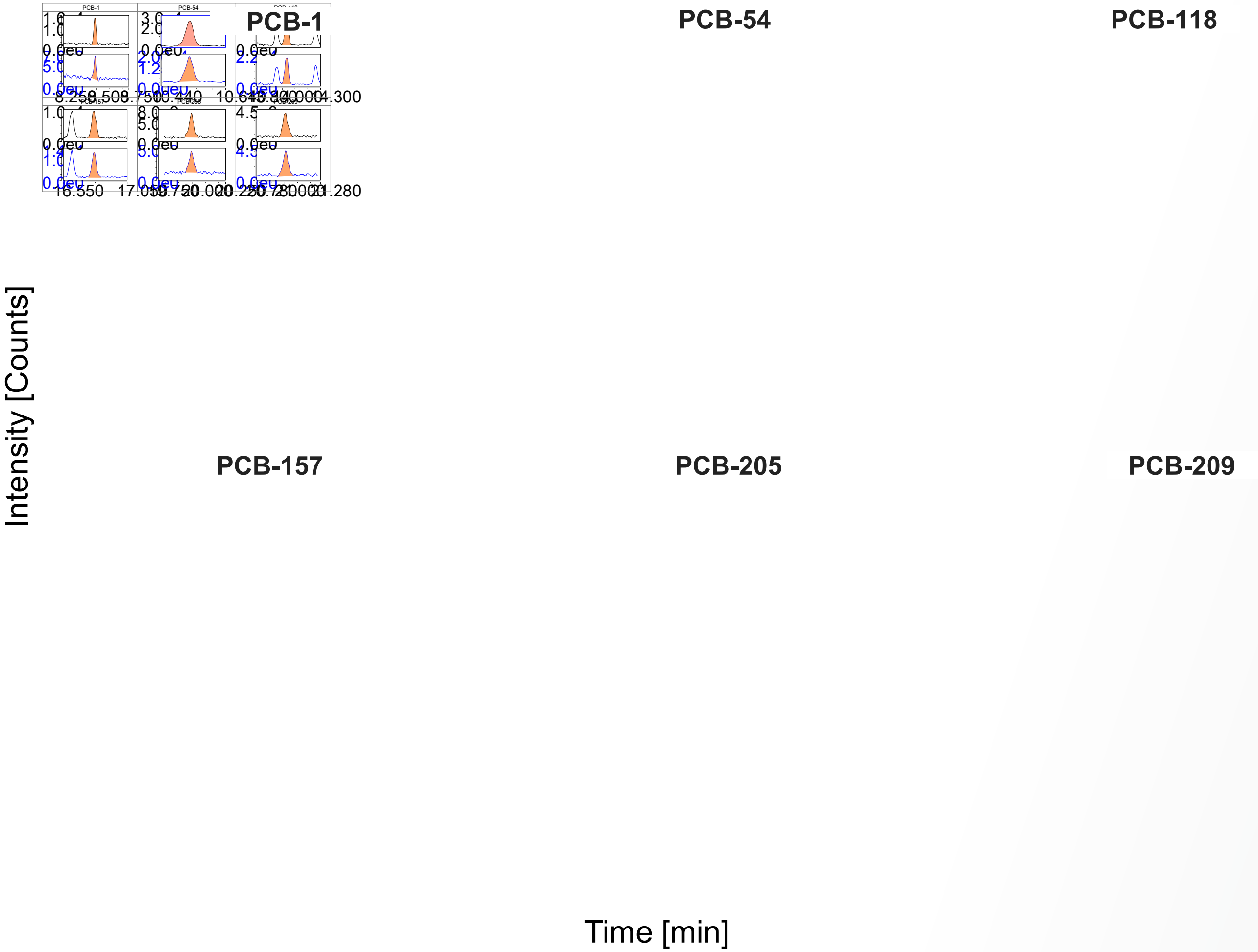
Compound	Retention Time (min)	Coefficient of determination (R^2)	AvCF %RSD
PCB-1	8.49	0.99993	1.5
PCB-3	9.03	0.99996	1.2
PCB-4	9.19	0.99987	2.1
PCB-19	9.88	0.99992	1.6
PCB-15	10.35	0.99996	1.2
PCB-54	10.53	0.99987	2.1
PCB-104	11.34	0.99987	2.1
PCB-37	11.83	0.99989	1.9
PCB-155	12.21	0.99168	17.3
PCB-77	13.40	0.99956	3.9
PCB-81	13.68	0.99925	5.0
PCB-188	13.80	0.99974	2.9
PCB-123	13.96	0.99967	3.3
PCB-118	14.04	0.99972	3.1
PCB-114	14.27	0.99962	3.6
PCB-105	14.74	0.99969	3.2
PCB-126	15.62	0.99990	1.9
PCB-202	15.67	0.99977	2.7
PCB-167	15.93	0.99707	10.0
PCB-156	16.62	0.99473	13.8
PCB-157	16.80	0.99437	14.3
PCB-169	17.84	0.99434	14.4
PCB-208	18.16	0.99991	1.8
PCB-189	18.90	0.99979	2.6
PCB-205	20.00	0.99960	3.6
PCB-206	20.57	0.99989	1.9
PCB-209	21.02	0.99978	2.7



andy.fornadel@thermofisher.com | 15-November-2022

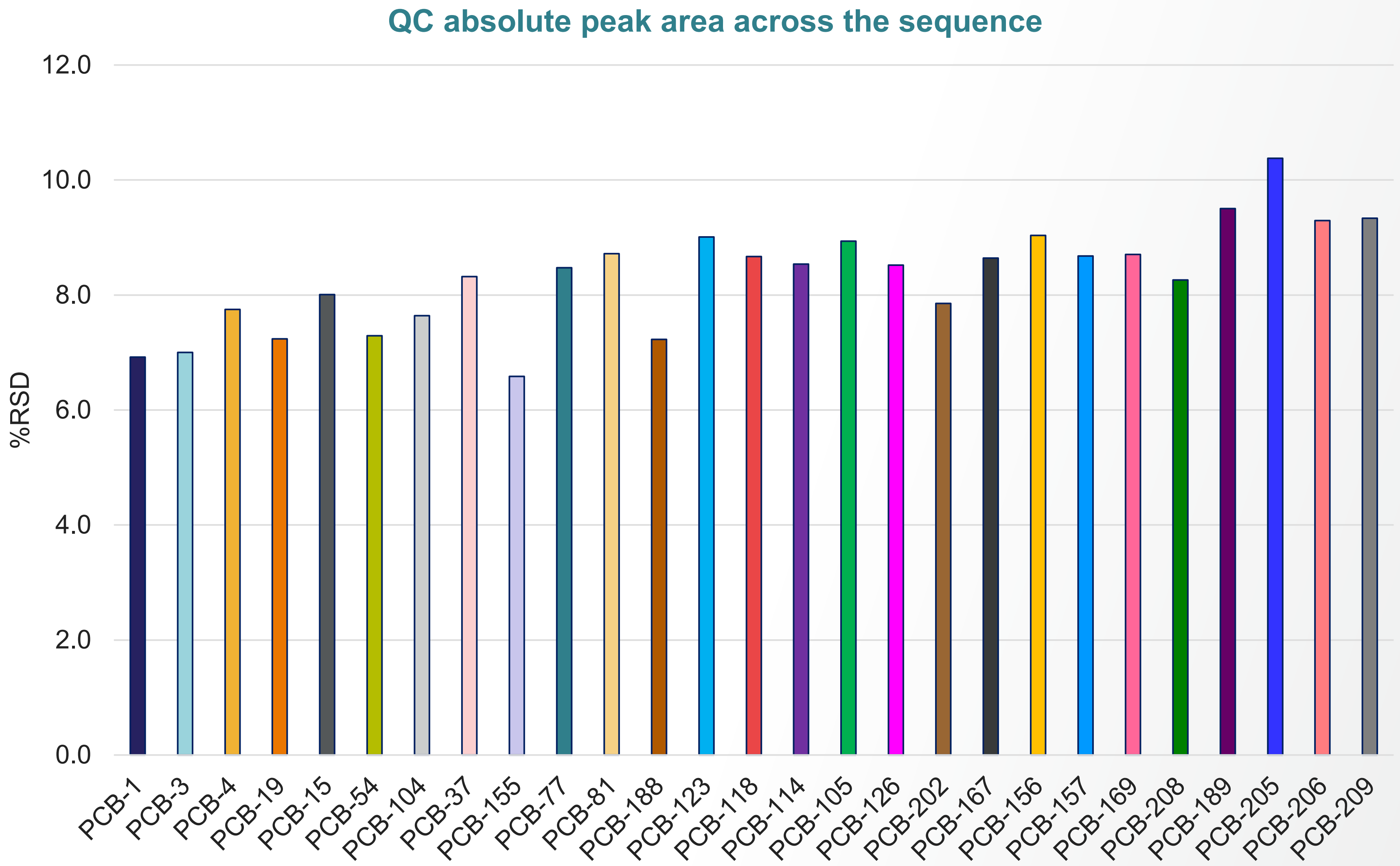
Assessment of sensitivity

LOQ = 0.05 ng/mL
(i) ion ratios within ± 15% the expected values
(ii) absolute peak area RSD <15%
(iii) the response factor (RF) RSD <15%



Compound	Absolute Peak Area %RSD (n=10)	RF %RSD	Expected IR	Average Measured IR (n=10)	Calculated IDL (fg OC)
PCB-1	2.2	2.4	33	33	3
PCB-3	4.1	4.3	33	35	6
PCB-4	5.4	5.2	64	65	8
PCB-19	2.8	2.9	62	67	4
PCB-15	2.9	2.3	64	67	4
PCB-54	1.8	2.8	64	65	3
PCB-104	7.3	6.3	95	99	10
PCB-37	2.4	2.4	61	63	3
PCB-155	13.5	6.5	124	123	19
PCB-77	3.0	1.9	63	66	4
PCB-81	3.1	2.9	63	65	4
PCB-188	6.4	6.2	157	148	9
PCB-123	7.5	7.5	102	94	11
PCB-118	4.1	3.5	101	96	6
PCB-114	4.9	4.1	96	97	7
PCB-105	4.8	5.7	95	93	7
PCB-126	13.0	11.6	90	83	18
PCB-202	5.4	6.6	64	66	8
PCB-167	4.8	5.3	123	119	7
PCB-156	10.5	8.2	123	130	15
PCB-157	9.1	5.4	122	128	13
PCB-169	5.9	10.4	129	132	8
PCB-208	9.9	6.6	98	98	14
PCB-189	11.2	10.9	154	151	16
PCB-205	8.0	6.4	64	64	11
PCB-206	8.8	6.2	97	98	12
PCB-209	8.8	6.6	110	111	12

Reproducibility



Compound	QC absolute peak area %RSD
PCB-1	6.9
PCB-3	7.0
PCB-4	7.7
PCB-19	7.2
PCB-15	8.0
PCB-54	7.3
PCB-104	7.6
PCB-37	8.3
PCB-155	6.6
PCB-77	8.5
PCB-81	8.7
PCB-188	7.2
PCB-123	9.0
PCB-118	8.7
PCB-114	8.5
PCB-105	8.9
PCB-126	8.5
PCB-202	7.9
PCB-167	8.6
PCB-156	9.0
PCB-157	8.7
PCB-169	8.7
PCB-208	8.3
PCB-189	9.5
PCB-205	10.4
PCB-206	9.3
PCB-209	9.3

Conclusions - PCBs

Thermo Fisher SCIENTIFIC

- The TRACE TR-PCB column ensured chromatographic separation of the target analytes in about 21 minutes with calculated resolution of the critical pair PCB-123 / PBDE-118 of 3%.
- The column thin film phase, high thermal stability, and low column bleed ensured elution of the high boiling point PCBs (e.g., PCB-209) with improved peak shapes.
- We demonstrated linearity over a concentration range of 0.10 to 2,000 ng/mL with coefficient of determination of R^2 >0.990 and AvCF %RSDs <20.
- IDLs ranged from 3 fg to 19 fg OC (corresponding to 0.15 pg/L to 0.95 pg/L in water samples and to 0.015 to 0.095 ng/kg in soil samples) and LOQ set at 0.05 ng/mL.
- Extended robustness demonstrated over 100 injections without need for maintenance or re-tuning.

Thank you