ThermoFisher
SCIENTIFIC

Environmental Capabilities

Richard F. Jack, Ph.D.
Sr. Director, Vertical Marketing – Environmental and Industrial

Our Business Segments

Analytical Instruments

Mass Spectrometry

Q-Exactive HF mass spectrometer

Chromatography

Vanquish Ultra HPLC

Chemical and Environmental Analysis

Gemini handheld analyzer

Life Science Solutions

Clinical Oncology

Next Gen Sequencing

Genetic Sciences

QuantStudio Dx R qPCR

Biosciences

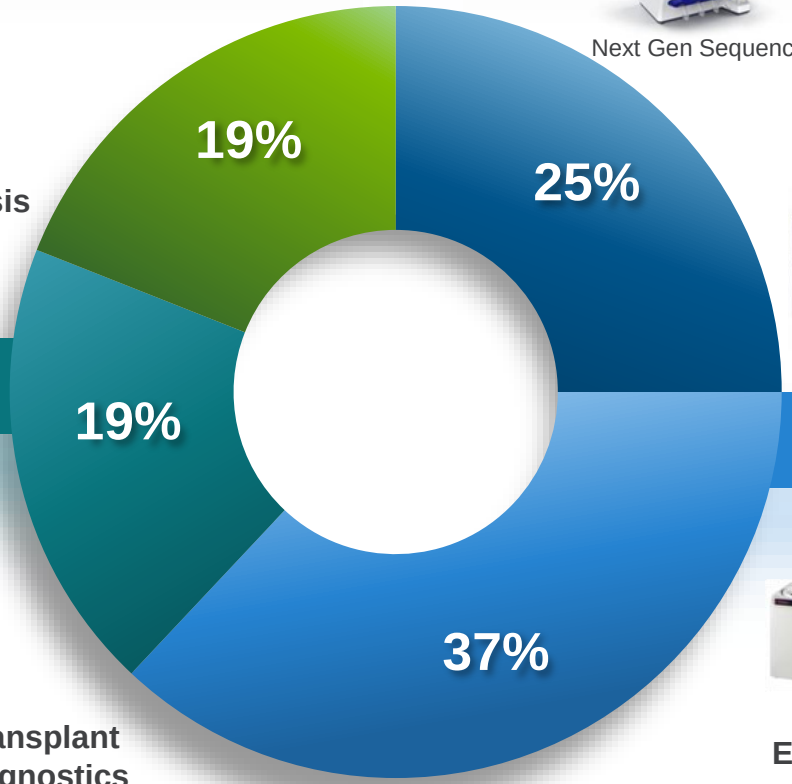
Life Science Reagents

Human Identification

GlobalFiler PCR Amplification Kit

BioProduction

Cell Culture Reagents



Specialty Diagnostics

ImmunoDiagnostics

ImmunoCAP Allergy and Asthma Tests

Clinical Diagnostics

Oral-Eze Oral Fluid Collection System

Microbiology

Antimicrobial Susceptibility Testing Solutions

Pathology

Rotary Microtome

Transplant Diagnostics

NXType High Resolution Genotyping

Laboratory Products and Services

Lab Equipment

Sorvall WX+ Ultracentrifuge

Distribution and BioPharma Services

Chemicals

Enterprise and Instrument Services

Lab Consumables

E1 ClipTip Pipette system

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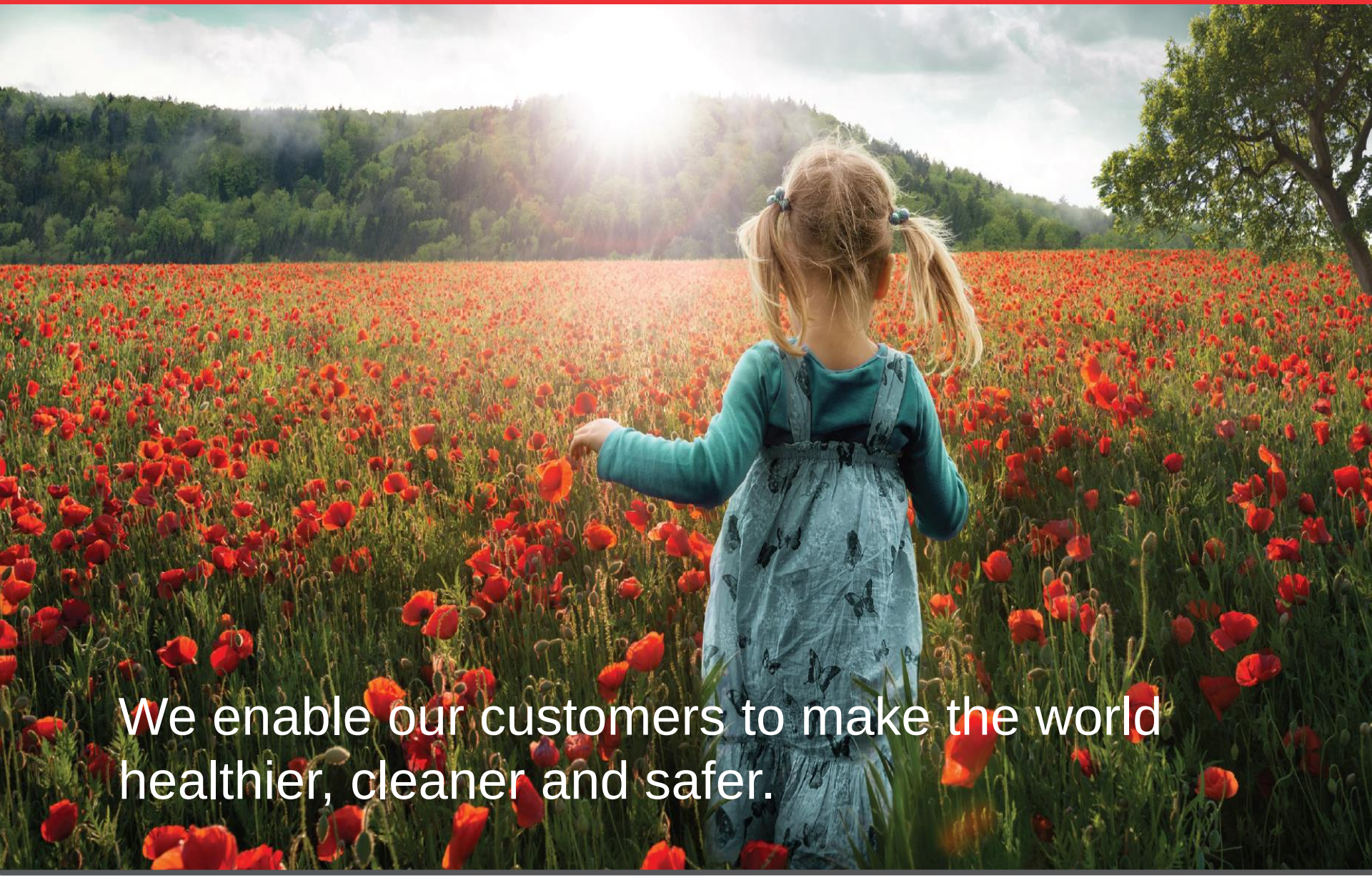
A Mission We are Proud of



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Our Environmental Capabilities

Ensuring Accuracy in Detection and Monitoring

- **World-class technological services** from sampling and data collection to reporting
- **Advanced methods** to test for microorganisms, chemical contaminants and radioactive and biological toxicity
- **Reliable results** for the laboratory, field and industrial processes
- **Analytical capabilities** at the point of need, to improve efficiency and reaction times

Maximizing Compliance Processes

- Deep regulatory compliance **knowledge and expertise**
- **Enhanced workflow efficiencies** for many different applications
- **Dedicated Center of Excellence** for researching and compliance support
- Timely technical **service and support**

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Environmental Contaminant Workflows

Comprehensive Contaminant Analysis Solutions

Sample Extraction

SPE

Dionex™ ASE™ 350 Accelerated Solvent Extractor

Dionex™ AutoTrace™ 280 Solid-Phase Extraction

Consumables

GC Columns & Consumables

LC Columns & Consumables

IC Columns & Consumables

Routine monitoring

GC, GCMS

LC, LCMS

IC, ICMS

Targeted & Non-Targeted monitoring

Orbitrap ™ GC-MS/MS

Orbitrap LC-MS/MS

Data analysis & Interpretation

SW & LIBRAIRIES

Laboratory Information Management Systems (LIMS)

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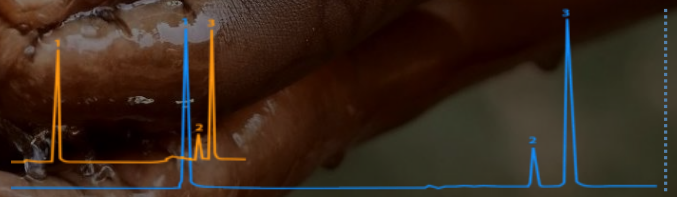
Ion Exchange Technologies

Extending Leadership in Ion Chromatography

Universal HPIC system

- HPIC extended from capillary column to microbore and standard analytical columns
- 5000 psi operation – just add water
- Faster, improved separations and higher resolution
- Reagent Free Ion Chromatography
- Always-on, always-ready capability



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New High Efficiency Dionex IonPac 4µm IC Columns in Analytical and Capillary Formats

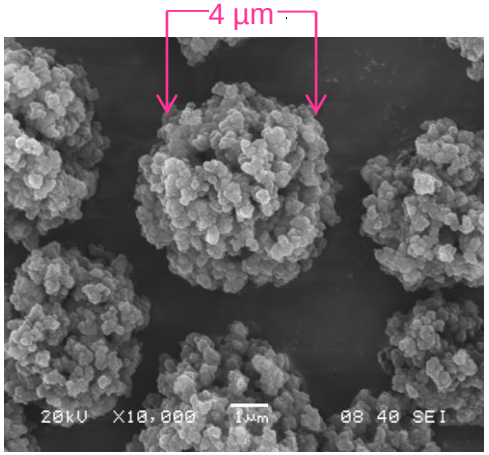
Ion-exchange columns with 4 µm particle-size

Benefits

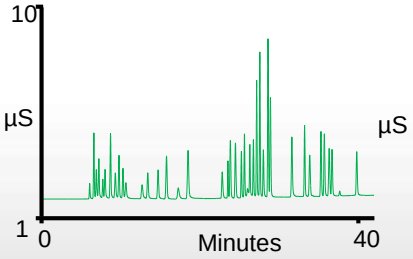
- Smaller particles provide better performance
- Faster run times with higher flow rates using 150 mm columns
- Better resolution with standard flow rates using 250 mm columns

Applications

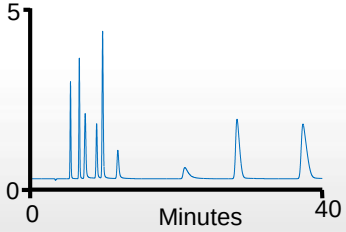
- Anions in environmental waters
- Organic acids in foods and beverages
- Amines in chemical process solutions



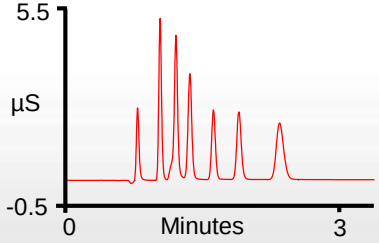
SEM Image of 4 µm Supermacroporous Bead



High Resolution using the Dionex IonPac AS11-HC-4µm



High Resolution using the Dionex IonPac CS19-4µm



Fast Run using the Dionex IonPac AS18-4µm

Improved Resolution Provides Faster Runs and Better Results

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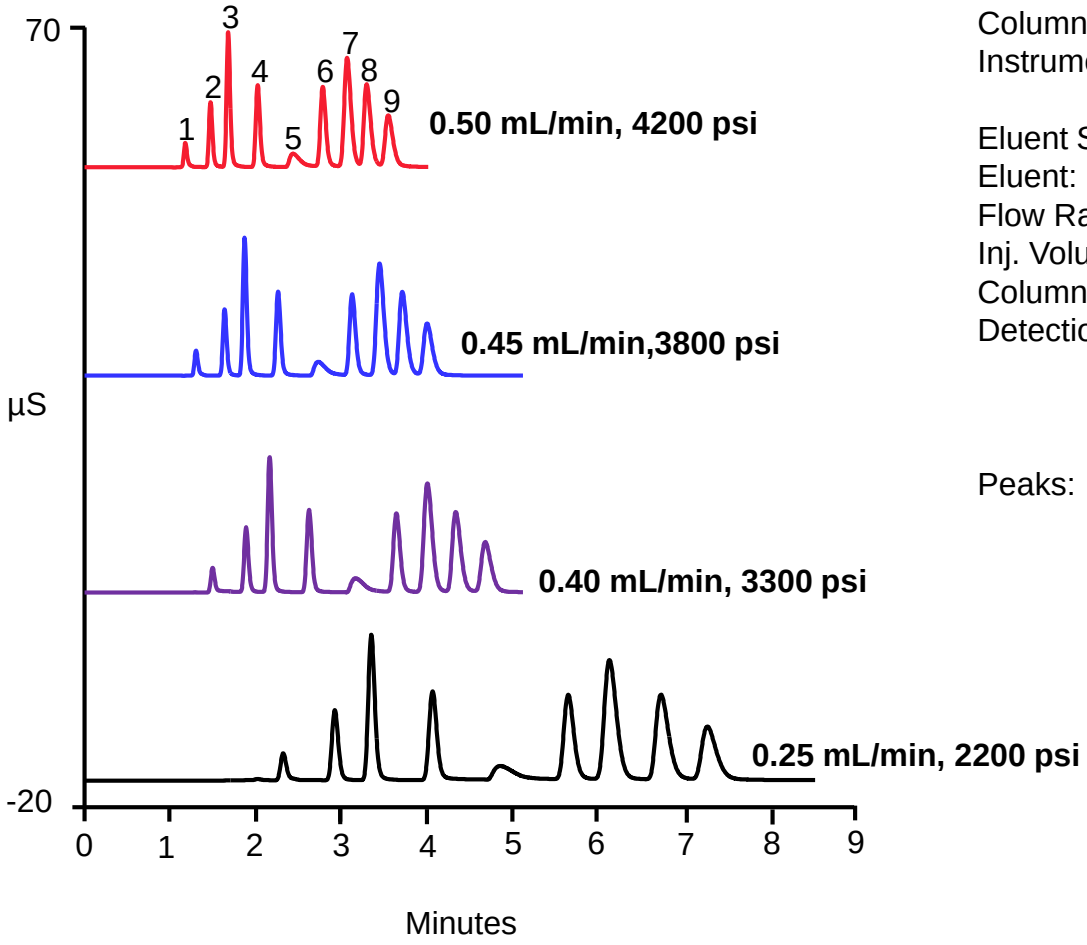
Faster Run Times without Sacrificing Resolution

Inorganic anions separation using a 4 µm Microbore column



Column:	Dionex IonPac AS18-4µm, 2 ×150 mm
Instrument:	Thermo Scientific™ Dionex™ ICS-5000⁺ HPIC™ System
Eluent Source:	Dionex EGC 500 KOH
Eluent:	23 mM Potassium hydroxide
Flow Rate:	0.25, 0.40, 0.45, and 0.50 mL/min
Inj. Volume:	5 µL
Column Temp.:	30 ° C
Detection:	Thermo Scientific™ Dionex™ ASRS™ 300 Anion Self-Regenerating Suppressor™, 2 mm, recycle

Peaks:			
	1. Fluoride	0.5	mg/L
	2. Chlorite	5.0	
	3. Chloride	3.0	
	4. Nitrite	5.0	
	5. Carbonate	20.0	
	6. Bromide	10.0	
	7. Sulfate	10.0	
	8. Nitrate	10.0	
	9. Chlorate	10.0	

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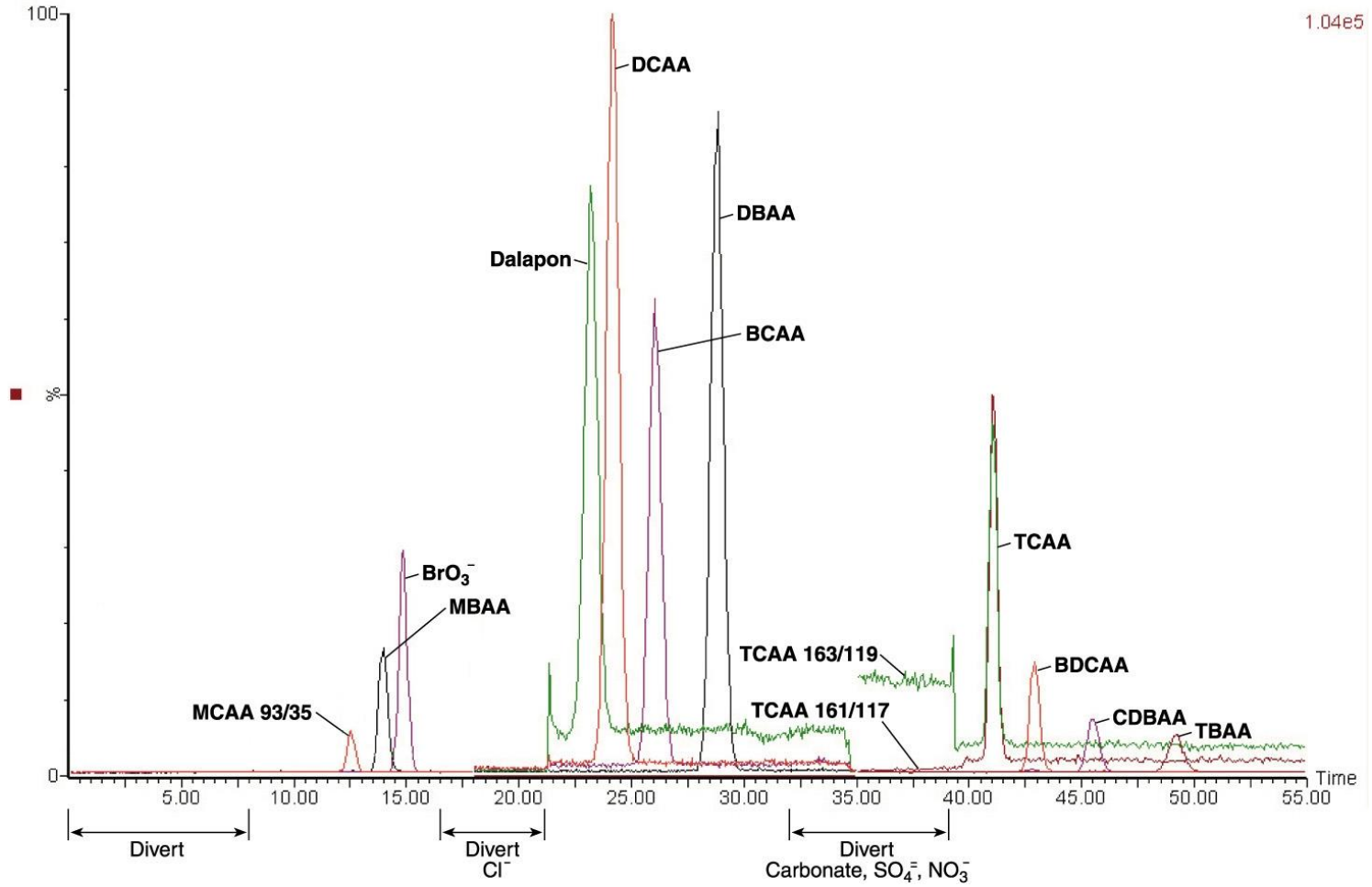
EPA 557: Determination of Bromate, Dalapon and HAA9 by Direct Injection using IC-MS/MS



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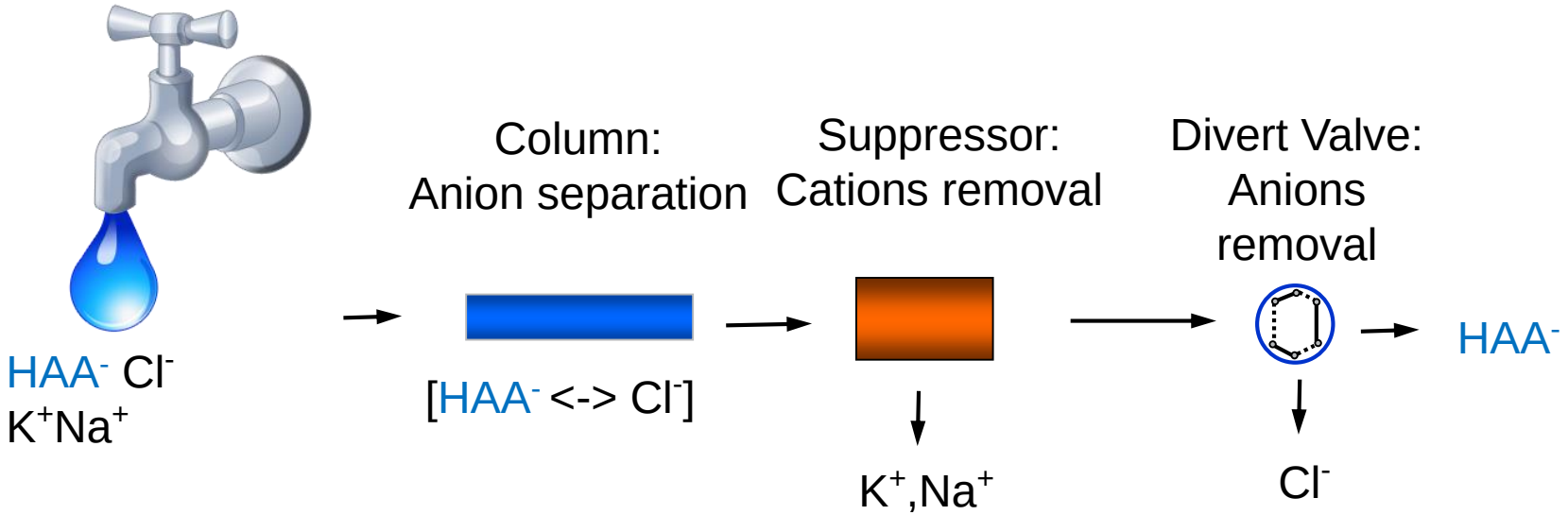
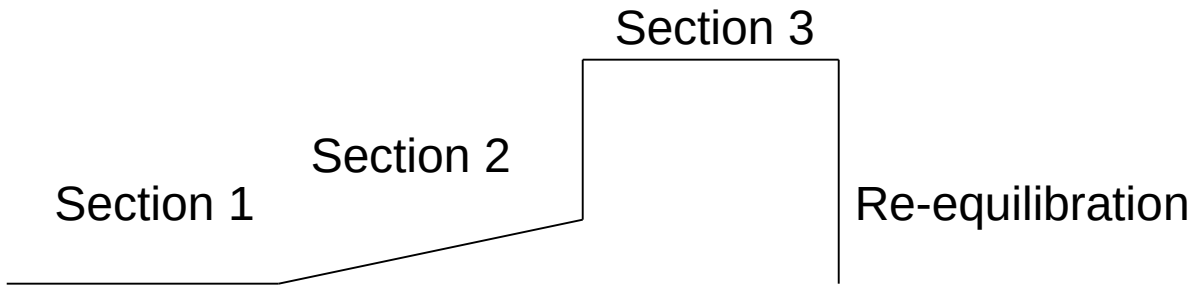
Matrix Elimination of Anions and Cations by Ion Exchange Chromatography



Strategy to eliminate signal suppression in the MS

Calibration: Isotope Dilution



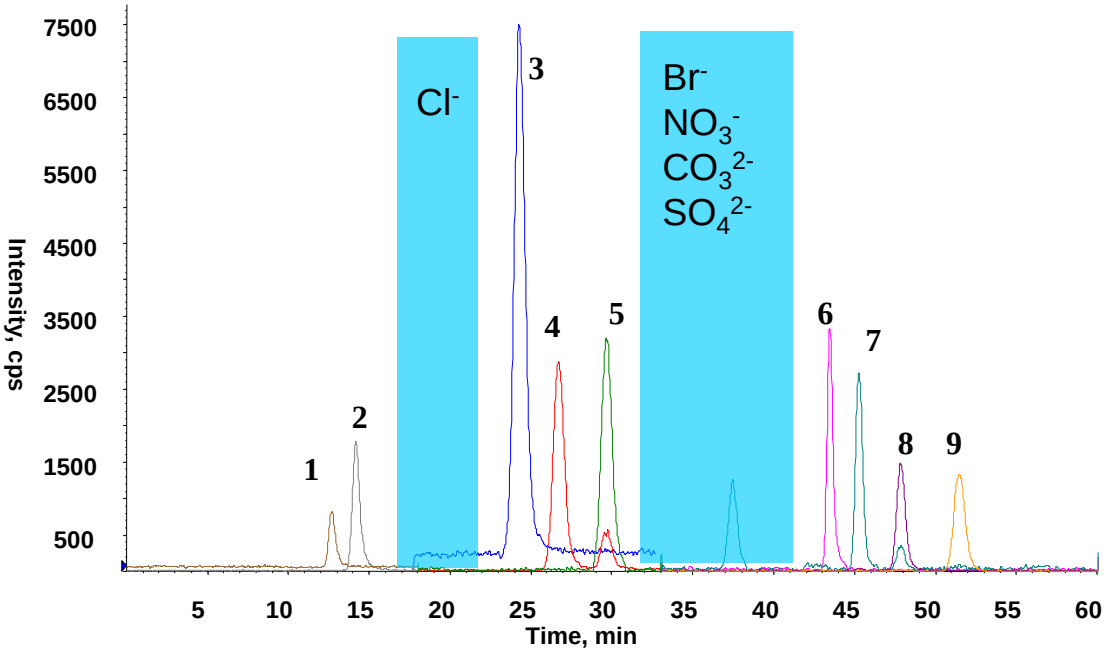
OH- Gradient

Internal Standards

MCAA-1-^{13}C
MBAA-1-^{13}C

DCAA-2-^{13}C

TCAA-2-^{13}C



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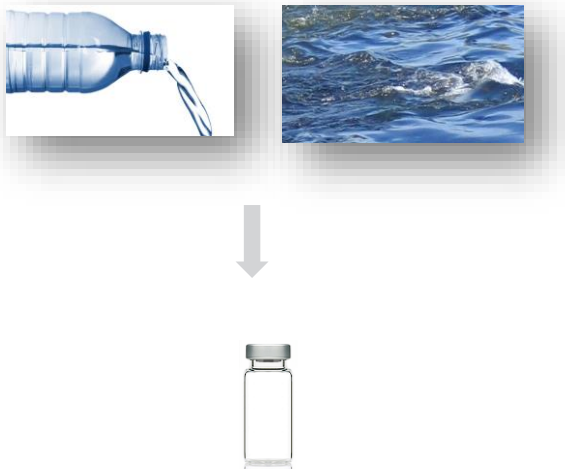
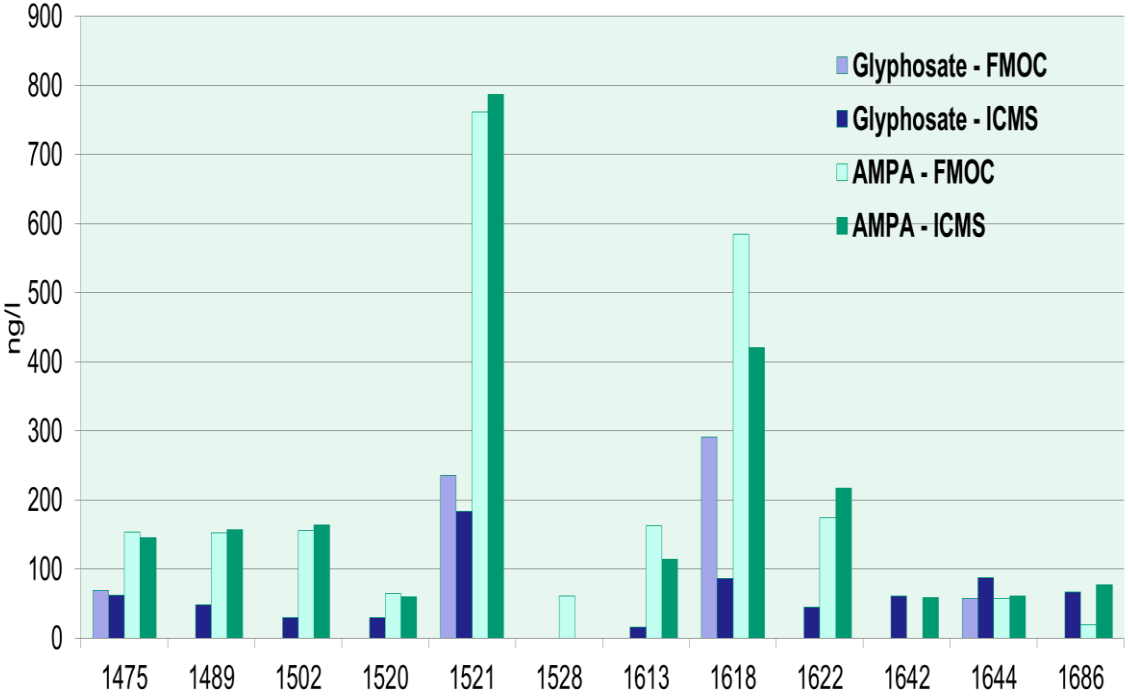
Ion Exchange for Ionic Pesticides comparison





- The IC-MS/MS compared to LC-MS/MS using FMOC derivatization:
- Direct injection without a long and laborious sample preparation
- More sensitive,
- Faster
- Fewer chances of sample manipulation errors.

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European Legislation for Perfluorinated Organics

Priority Substances listed in directive 2013/39/EU with Priority Hazardous Substances in bold

Alachlor	**Hexachlorobenzene**	Trichlorobenzenes
Anthracene	**Hexchlorobutadiene**	Trichloromethane (chloroform)
Atrazine	**Hexachlorocyclohexane**	**Trifluralin**
Benzene	Isoproturon	**Dicofol**
Brominated diphenylethers	Lead and its compounds	**Perfluorooctane sulfonic acid and its derivatives (PFOS)**
Cadmium and its compounds	**Mercury and its compounds**	**Quinoxyfen**
Chloroalkanes, C_{10-13}	Naphthalene	**Dioxins and dioxin-like compounds**
Chlorfenvinphos	Nickel and its compounds	Aclonifen
Chlorpyrifos (Chlorpyrifos-ethyl)	**Nonylphenols**	Bifenox
1,2-dichloroethane	Octylphenols	Cybutryne
Dichloromethane	**Pentachlorobenzene**	Cypermethrin
Di (2-ethylhexyl) phthalate (DEHP)	Pentachlorophenol	Dichlorvos
Diuron	**Polyaromatic Hydrocarbons (PAH)**	**Hexabromocyclododecanes (HBCDD)**
Endosulfan	Simazine	**Heptachlor and Heptachlor epoxide**
Fluoranthene	**Tributyltin compounds**	Terbutryn

- We are seeing more of a global interest for PFC's.
- Contract labs in EU are looking for the most sensitive methods
- US an increased interest in branched and degradation products.
  - No standards are available
  - HRAM using Orbitrap is the preferred tool.

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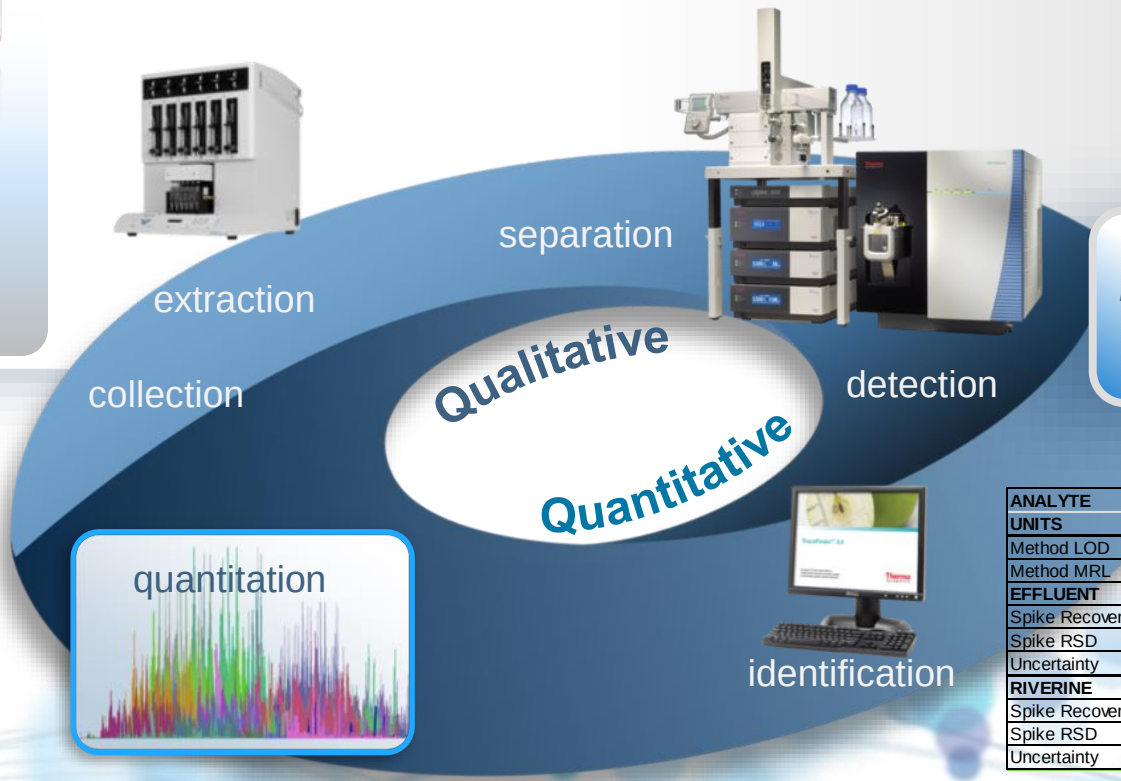
Case Study: Perfluorinated Organics in Drinking Water

Dr. Andy Eaton
Technical Director
Eurofins Eaton

"The HRAM performance has better sensitivity than LC-MS/MS for EPA 537 with additional confirmation such as product ions and a spectral library match."

Targeted and Non-Targeted Analysis



ng/L sensitivity for known and unknown perfluorinated compounds.

ANALYTE	PFOS	PFOA
UNITS	ng/L	ng/L
Method LOD	0.0676	0.0539
Method MRL	0.09	0.09
EFFLUENT		
Spike Recovery	96.9%	94.8%
Spike RSD	4.15%	2.38%
Uncertainty	11.41%	10.00%
RIVERINE		
Spike Recovery	94.4%	95.9%
Spike RSD	5.53%	5.17%
Uncertainty	16.65%	14.47%

Complete solutions, from qualitative to quantitative

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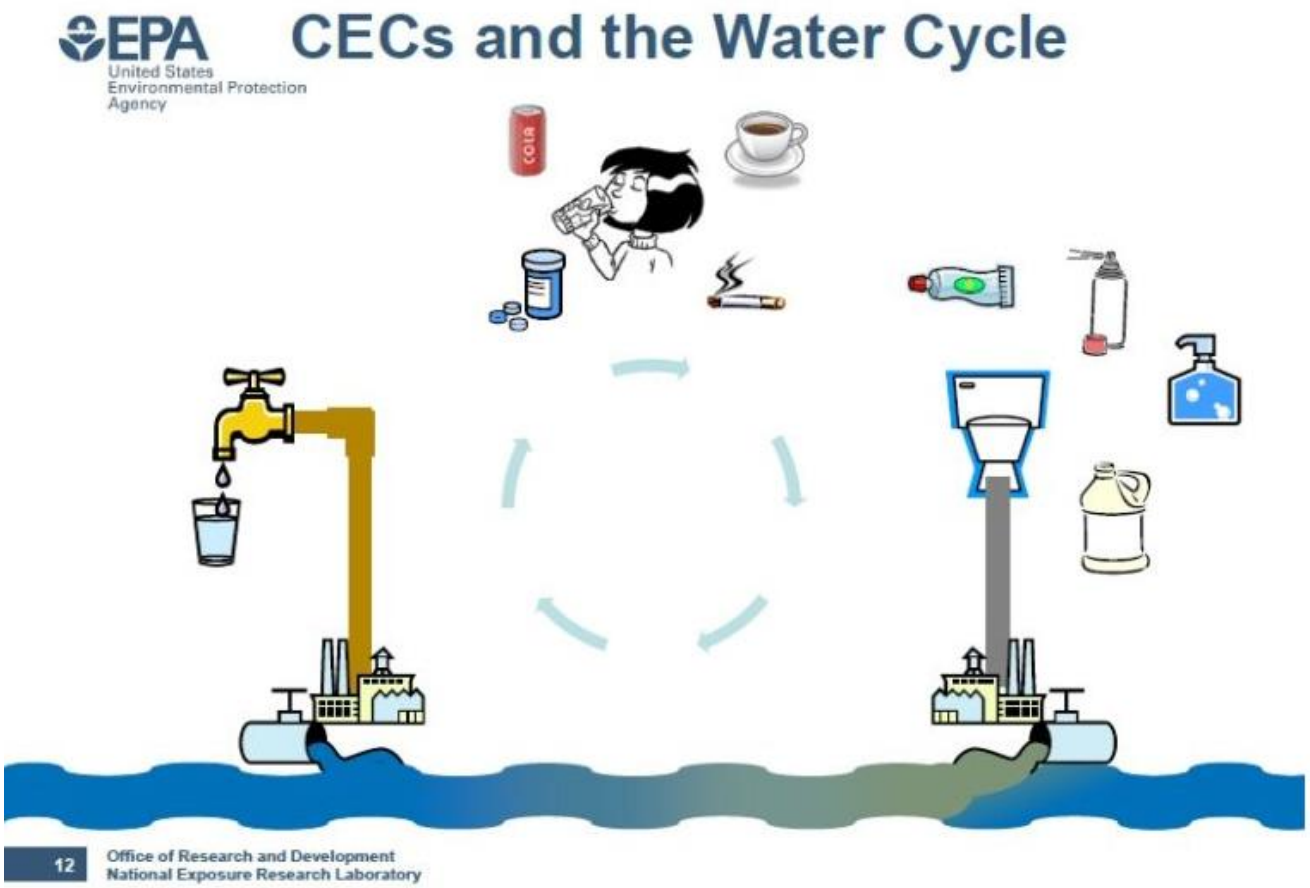
Environmental Industry Trends

- The path from “Emerging Contaminants” to “Regulated Contaminants”



U.S. Environmental Protection Agency graphic

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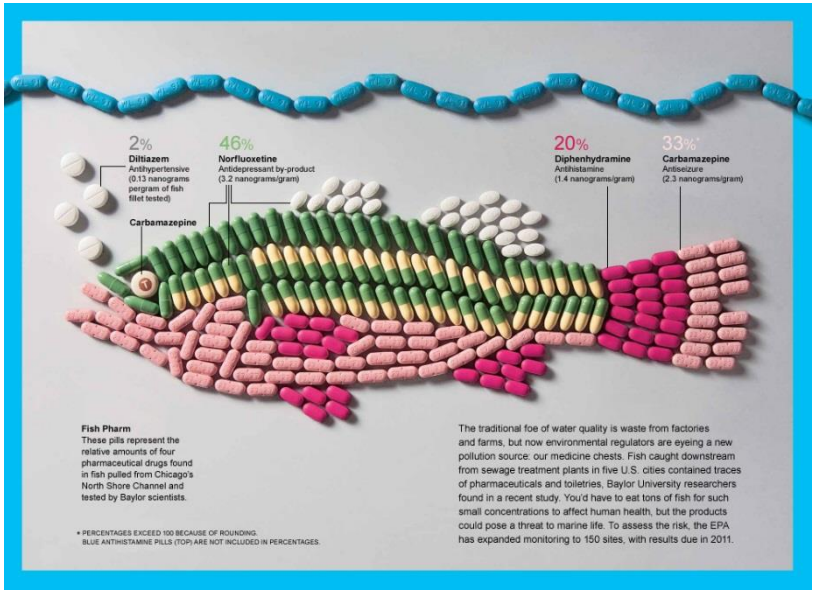
PPCPs and endocrine disruption



Pharmaceuticals, Personal Care Products, Pesticides
*Image from *National Geographic, April 2010*

News
European Parliament

Identifying endocrine disruptors: Parliament blocks plans exempting some pesticides

Press Releases | PLENARY SESSION | ENVI | 04-10-2017 - 13:45

EPA United States Environmental Protection Agency

Endocrine Disruptor Screening Program (EDSP)

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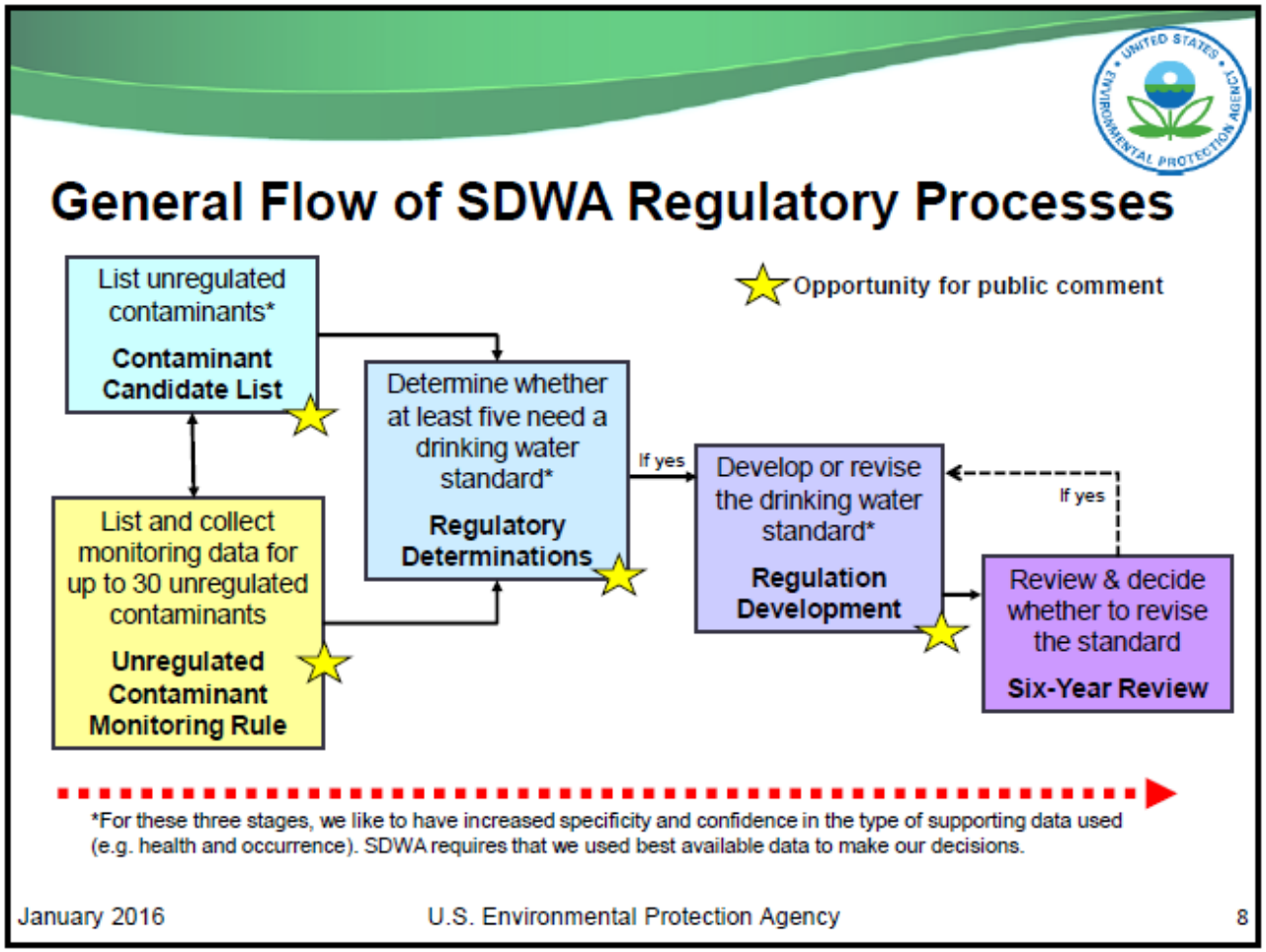
Drinking Water: Process Unregulated Contaminant Monitoring Rule



- CCL3 approx.. 7500 > 100
- Issue no more than 30 every 5 years

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EPA OGWDW Methods For PFC's and Hormones

- Method 537: *Determination of Selected **Perfluorinated Alkyl Acids** in Drinking Water by Solid Phase Extraction and Liquid Chromatography/ Tandem Mass Spectrometry*

- Method 539: *Determination of **Hormones** in Drinking Water by Solid Phase Extraction and Liquid Chromatography Electrospray Ionization Tandem Mass Spectrometry*
  - *Includes man made*

- Both methods have a targeted list of compounds
  - Represent a broad array of compounds
  - But are they the right list?

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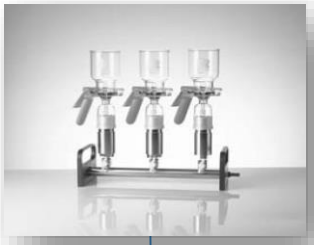
DW contaminant approach

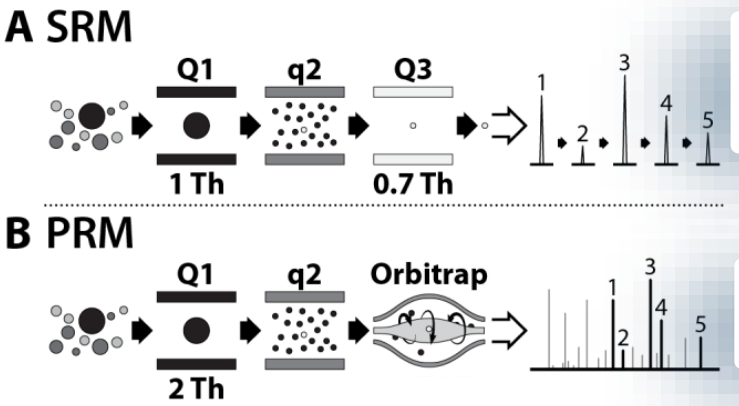


QQQ

Orbitrap®

Using EPA 537 and 539 we want to:

1. Develop automated SPE
2. Compare quantitation between MS/MS with Orbitrap
3. Search for unknowns…



Serial monitoring

Parallel monitoring

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Manual vs. Automated SPE

- **Silica Based SPE Cartridges**
  - SolEx C8
  - SolEx C18
  - SolEx C8-clean (phthalate-free)
  - SolEx C18-clean (phthalate-free)
  - SolEx C18-525
  - SolEx unbonded silica
- **Carbon Based SPE Cartridges**
  - SolEx activated carbon
  - SolEx graphitized carbon
- **Polymeric New SolEx Phases**
  - SolEx HRPHS → Hydrophilic, reversed phase column
    - Specifically developed for water soluble PPCP's
  - SolEx SAX
  - SolEx SCX
  - SolEx WAX
  - SolEx WCX
- **InLine SolEx Cartridges**
  - SolEx HRPHS

Demonstrated equivalency to manual SPE

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EPA 537 Method Used - Summary

- A 250-mL preserved water sample with Trizma is fortified with surrogates and passed through a solid phase extraction (SPE) cartridge containing Solex HRPHS in leu of polystyrenedivinylbenzene (SDVB) to extract the method analytes and surrogates. The compounds are eluted from the solid phase with a small amount of methanol. The extract is concentrated to dryness with nitrogenin a heated water bath, and then adjusted to a 1-mL volume with 96:4% (vol/vol) methanol:water after adding the IS(s). A 5-µL in leu of 10-µL injection is made into an LC equipped with a C18 column that is interfaced to an

- Q-Exactive hybrid HRAM capable of producing MS/MS data in leu of “low resolution triple” - MS/MS. The analytes are separated and identified by comparing the acquired mass spectra and retention times to reference spectra and retention times for calibration standards acquired under identical LC/MS/MS conditions. The concentration of each analyte is determined by using the internal standard technique. Surrogate analytes are added to all Field and QC Samples to monitor the extraction efficiency of the method analytes.

30

1. Detection Limit comparison

	MS/MS		Orbitrap	
Method 539 UCMR3 Analyte	MRL (ng/L)	LCMRL[a] (ng/L)	LCMRL (ng/L)	DL (ng/L)
17α-ethynylestradiol	0.9	1.3	< 0.05	0.1
17β-estradiol	0.4	0.32	0.17	0.047
equilin	4	0.28	< 0.23	0.48
estriol	0.8	3	0.27	0.2
estrone	2	4	0.84	0.48
testosterone	0.1	0.062	0.033	0.027
androstenedione	0.3	0.37	0.19	0.08

[a]The LCMRL is the lowest spiking concentration with recovery between 50 and 150 percent is expected 99 percent of the time by a single analyst.

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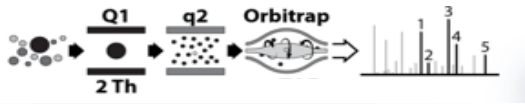
What unknowns are present in “Hormone” extracts?

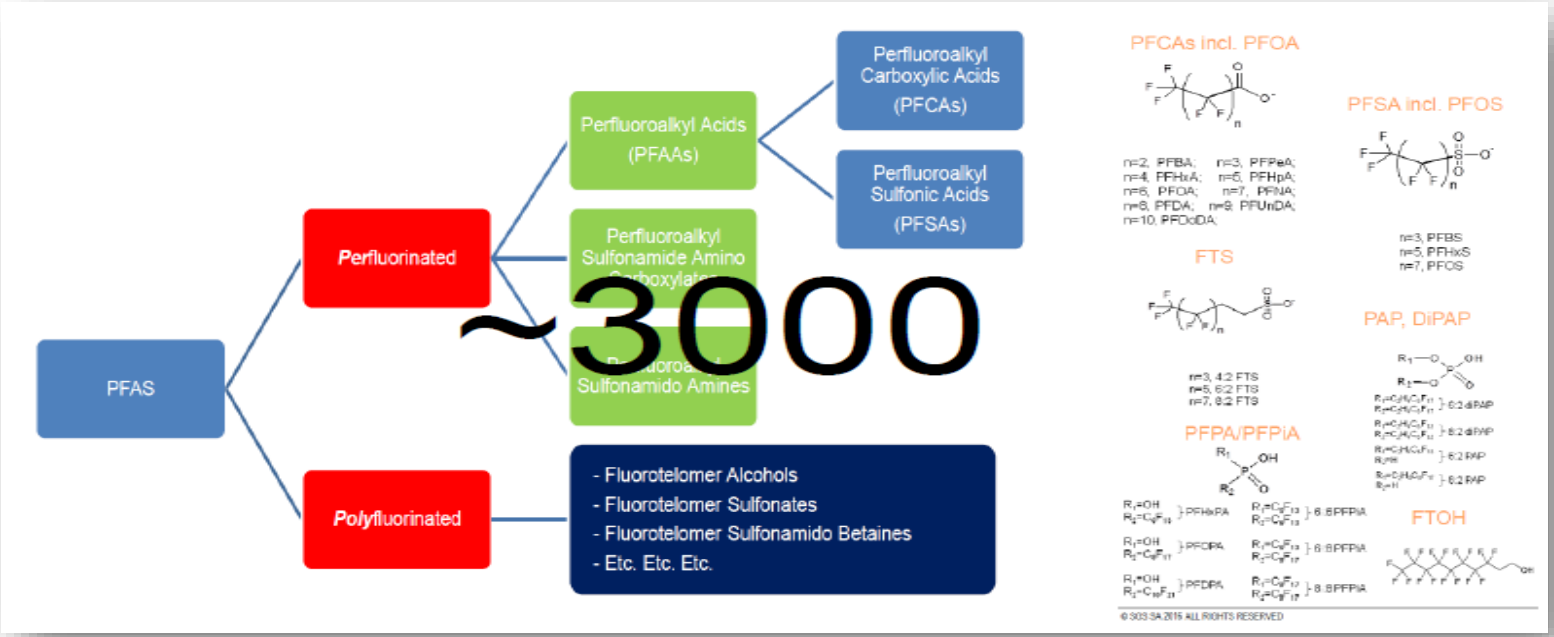
2. EPA 539 extract results using Full Scan monitoring

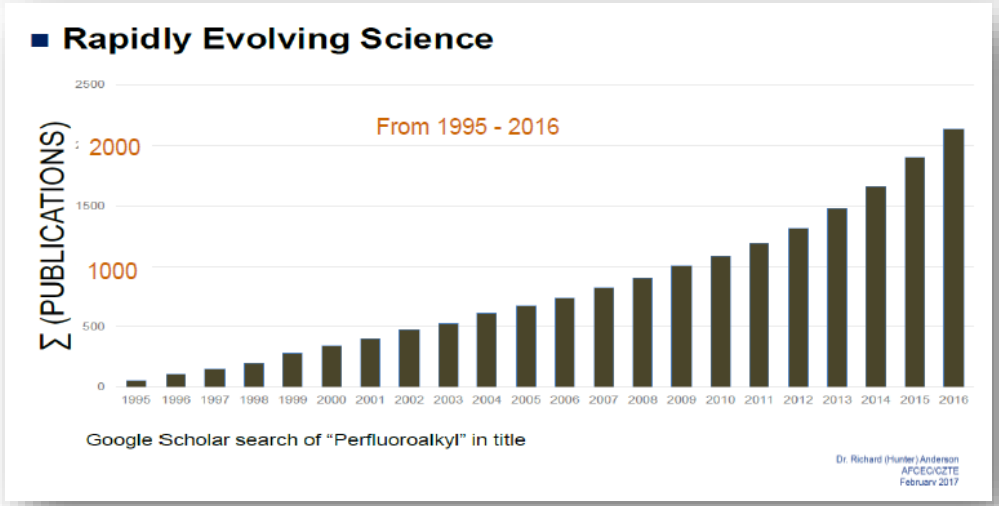


***Full Scan mon**nitoring*

ID	CompMW	Formula	MZ	Time	HitCount				
CSID	Name	Formula	SMILES	MW	AvgMass	MonoisotopicMass	SearchMass	DeltaPPM	Adduct
14620	**Atraton**	C_{9}H_{17}N_{5}O	CC/N=c/1\[nH]/c(=N/C(C)C)/[nH]c(n1)OC	211.2642	211.2642	211.143311	211.1428815	2.03436459	comp
11	232.016676	C1H5O9N5	231.0093994	7.780558586	1				
DetailTable: 1 Items									
CSID	Name	Formula	SMILES	MW	AvgMass	MonoisotopicMass	SearchMass	DeltaPPM	Adduct
3008	**Diuron**	C_{9}H_{10}Cl_{2}N_{2}O	CN(C)/C(=N\c1ccc(c(c1)Cl)Cl)/O	233.0945	233.0945	232.017014	232.016676	1.45673122	comp
12	234.1254712		233.1181946	5.222514153	2				
DetailTable: 2 Items									
CSID	Name	Formula	SMILES	MW	AvgMass	MonoisotopicMass	SearchMass	DeltaPPM	Adduct
4E+06	**Stiripentol**	C_{14}H_{18}O_{3}	CC(C)(C)C(/C=C/c1ccc2c(c1)OCO2)O	234.29092	234.2909	234.125595	234.1254712	0.528861389	comp

Perfluorinated Compounds as Emerging Contaminants





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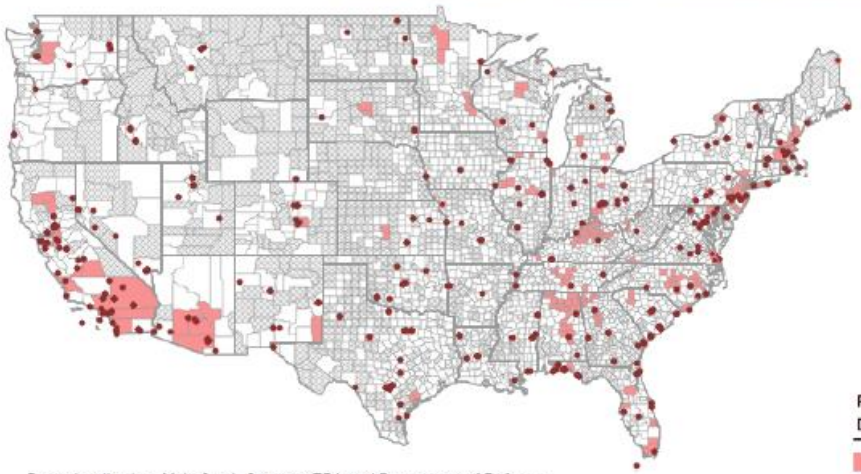
US DW survey results : PFC's

- HITS for targeted PFC's in the US, UCMR3
- Targeted suspects only, but what else is present in the same DW extracts?

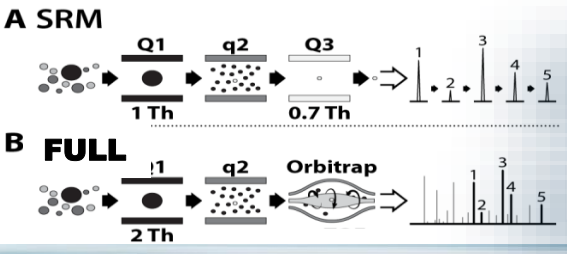
2012: Six PFASs added to Unregulated Contaminant Monitoring Rule 3 (UCMR 3) list, including PFOS and PFOA using EPA 537 method.

October 2015 UCMR 3 data summary



Data visualization: Moiz Syed. Sources: EPA and Department of Defense.
https://theintercept.com/2015/12/16/toxic-firefighting-foam-has-contaminated-u-s-drinking-water-with-pfcs/

Contaminant	Minimum Reporting Level
PFOS	0.04 µg/L
PFOA	0.02 µg/L
PFNA	0.02 µg/L
PFHxS	0.03 µg/L
PFHpA	0.01 µg/L
PFBS	0.09 µg/L



Serial monitoring

Full Scan monitoring

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EPA 537: Comparing PFC Quantification MS/MS with Orbitrap

1. Detection Limit comparison

LCMRL equal or better than high end - mid range triple quads – background contamination is the limiting factor.

PRM

	DL	LCMRL
PFBS	0.12	<0.5
PFDA	<0.5	<0.5
PFDoA	0.29	<0.5
PFHpA	0.35	0.97
PFHxA	0.27	<0.5
PFHxS	0.52	0.77
PFNA	0.26	<0.5
PFOA	0.36	0.5
PFOS	0.21	<0.5
PFTA	0.48	0.71
PFTrDA	0.32	<0.5
PFuNA	0.31	0.72

Full Scan

	DL	LCMRL
PFBS	0.2	<0.5
PFDA	0.26	<0.5
PFDoA	0.47	0.73
PFHpA	0.15	<0.5
PFHxA	0.19	<0.5
PFHxS	1.7	2.4
PFNA	0.17	<0.5
PFOA	0.22	0.5
PFOS	0.26	0.5
PFTA	0.2	<0.5
PFTrDA	0.31	0.55
PFuNA	0.38	1
PFBA	0.19	0.64
PFODA	0.55	1
PFDS	0.19	<0.5
PFHxDA	0.12	0.5
PFPA	0.19	<0.5

Stock standard contained other compounds not part of EPA 537 target list which were identified and quantified using Full-MS

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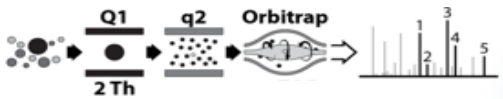
Unknown PFC's using Orbitrap Technology

2. EPA 537 PFC extract results using Full Scan monitoring

- Compared to library of ~75 PFCs and related compounds
- All 5 had at least 1 UCMR3 detect
- In addition we found several had unknown per and polyfluorinated compounds
- All have mass errors of < 3 ppm ie., highly accurate identification

Unknowns found in EPA 537 Extracts using Full Scan	
PFHPS	6:2 diPAP
PFDS – 10:2 FTOH	
8:2 FTA	
2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate	
PFDOA	
PFHxDA	



Full Scan monitoring

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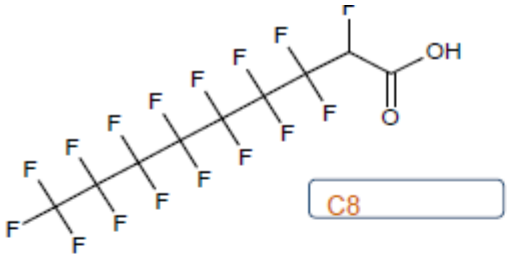
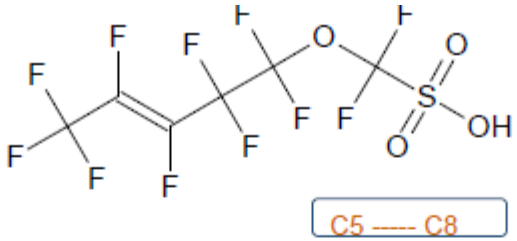
Finding Emerging PFC's using HRAM



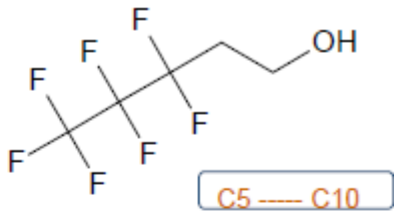
C8

hexadecafluorononanoic acid



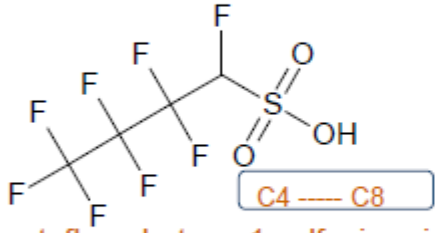
C5 ----- C8

difluoro{[(3E)-1,1,2,2,3,4,5,5,5-nonafluoropent-3-en-1-yl]oxy}methanesulfonic acid



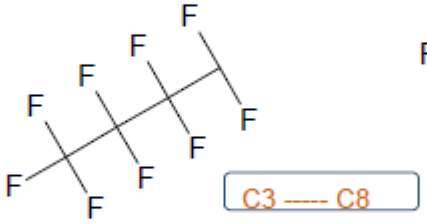
C5 ----- C10

3:2 FTOH



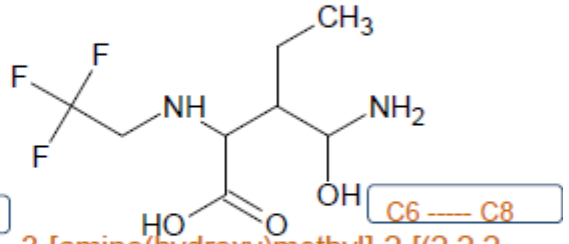
C4 ----- C8

octafluorobutane-1-sulfonic acid



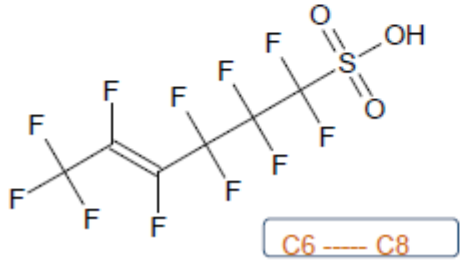
C3 ----- C8

nonafluorobutane



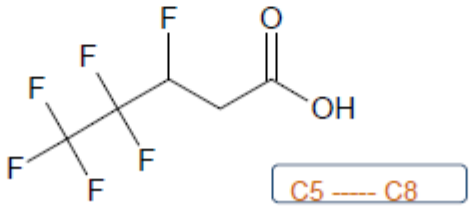
C6 ----- C8

3-[amino(hydroxy)methyl]-2-[(2,2,2-trifluoroethyl)amino]pentanoic acid



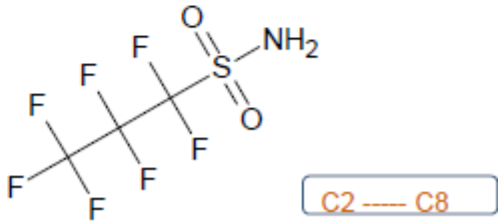
C6 ----- C8

undecafluorohex-4-ene-1-sulfonic acid



C5 ----- C8

3:2 FTA



C2 ----- C8

heptafluoropropane-1-sulfonamide

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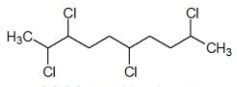
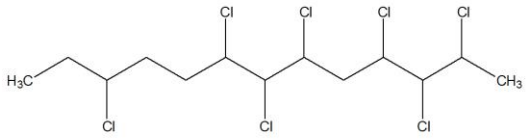
Introduction to chlorinated paraffins (CP)

- Emerging POPs consisting of **short** (C_{10}-C_{13}), **medium** (C_{14}-C_{17}) or **long** (>C_{17}) chain polychlorinated n-alkanes with toxic effects on human health and the environment.
- Persistence and believed harmful effects on exposed humans/environment place SCCPs on Stockholm Convention POPs candidate list; **added to Annex A in April/May 2017** (COP.8 decision).
- Mainly used in manufacturing of sealants, flame retardants, in leather processing, paints and coatings, metal working fluids.
- Manufacturing of SCCPs is in Europe regulated (ex: directive 2002/45/EC, Regulation EU 519/2012) and limits for usage are set (Regulation EU 2015/2030).
- Annual CP production >1.1 million tonnes*, similar to the total production volume of PCBs.



2,3,6,9-tetrachlorodecane Composition = C(42.89%) H(6.48%) Cl(50.64%)



2,3,4,6,7,8,11-heptachlorotridecane Composition = C(36.70%) H(4.97%) Cl(58.33%)

* Glüge J, Wang Z et al (2016) *Science of the Total Environment,* **573** 1132–1146

EURL European Union Reference Laboratory Dioxins and PCBs

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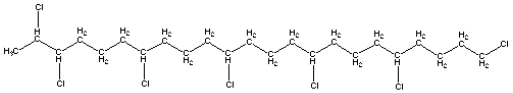
Persistant Organic Pollutants

- Incineration products
  - Polychlorinated dibenzodioxins –PCDDs (75)
  - Polychlorinated dibenzofurans - PCDFs (135)

- Environmental contaminants
  - Polychlorinated biphenyls – PCBs (209)
  - Polybrominated diphenyl ethers – PBDEs (209)
  - **Chlorinated paraffins**
  - Organochlorine pesticides
  - Polyfluorinated ether sulphones

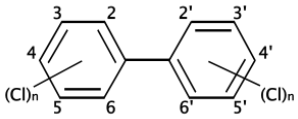
Chlorinated Paraffins



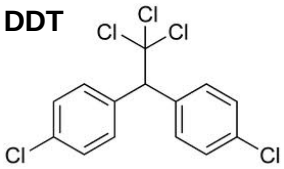
Large numbers of cogeners but of differing toxicity

High specificity is required to focus on toxicologically significant POPs

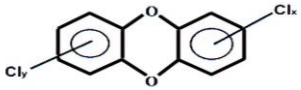
Polychlorinated biphenyls



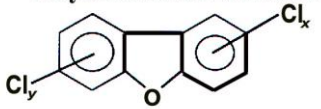
DDT



Polychlorodibenzo-p-dioxin



Polychlorodibenzofuran



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Q Exactive GC Orbitrap GC-MS/MS system: The technology inside

Orbitrap mass analyzer

Incredible HRAM performance

Highly regarded Thermo Scientific™ Q Exactive GC Orbitrap™ GC-MS/MS system platform

Thermo Scientific™ TRACE™ 1310 GC System

Unique modular injector and detector design

Rapid heat cycling

Thermo Scientific™ ExtractaBrite™ Ion Source technology

Routine grade robustness

Patented RF lens

Removable without breaking vacuum

EURL European Union Reference Laboratory Dioxins and PCBs

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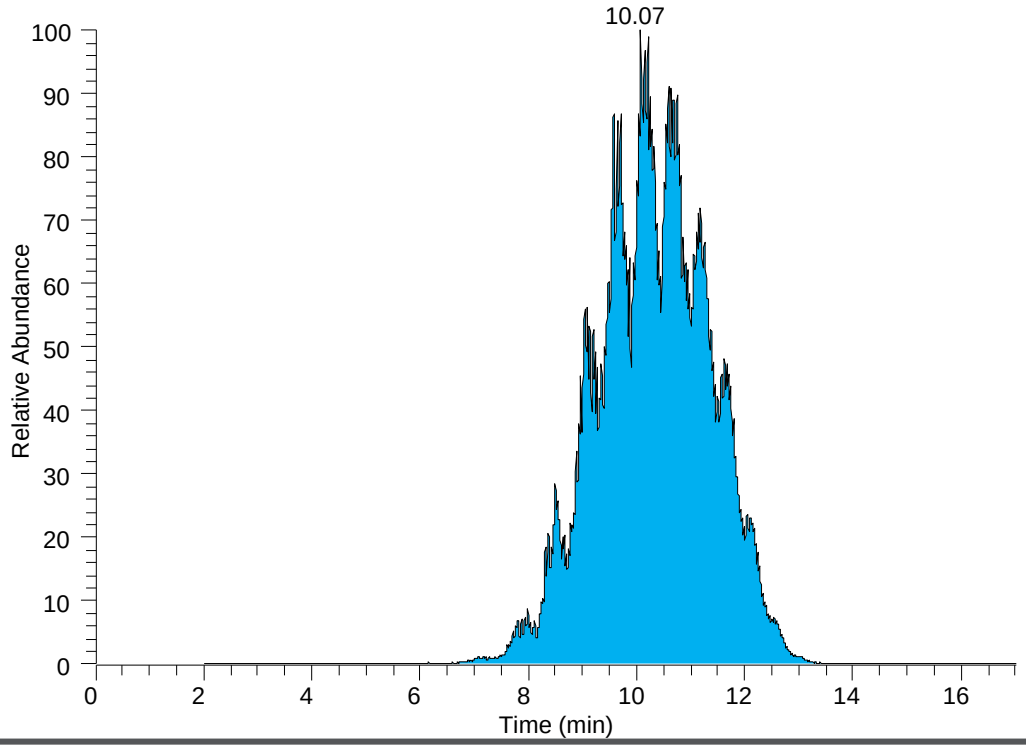
Analytical challenges

- Currently there is no consensus for the use of a validated analytical procedure for routine monitoring of CPs in food and feed.

- SCCPs and MCCPs have thousands of homologues and isomers that cannot be separated chromatographically. This, together with low concentrations makes their detection and quantification difficult.



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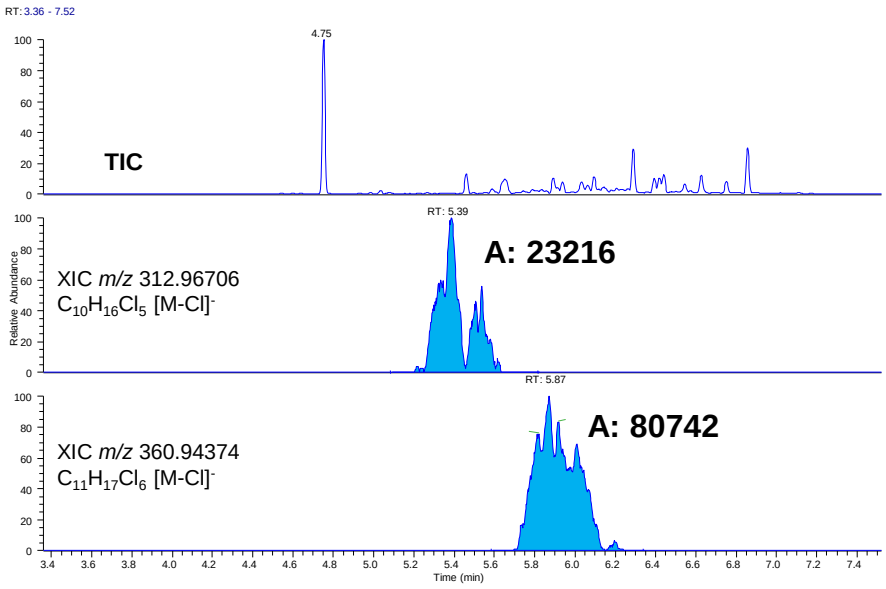
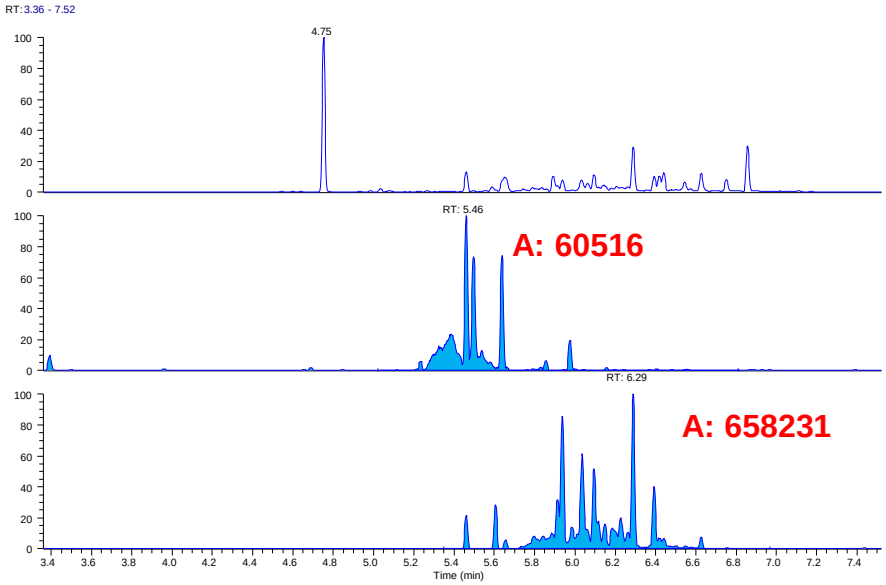
Selectivity through high resolving power

- By using high resolution GC-MS the risk of overestimating the CP content due to interferences from other CPs or halogenated compounds such as PCBs is reduced.

±3 ppm mass window



nominal mass window



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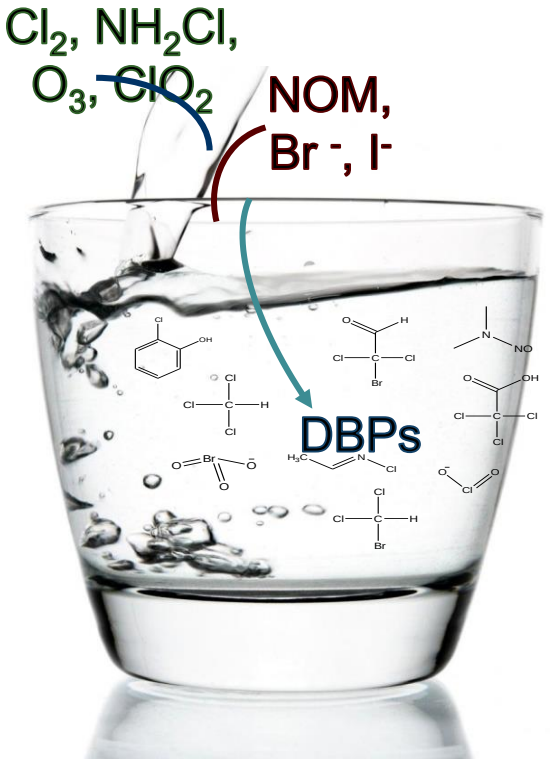
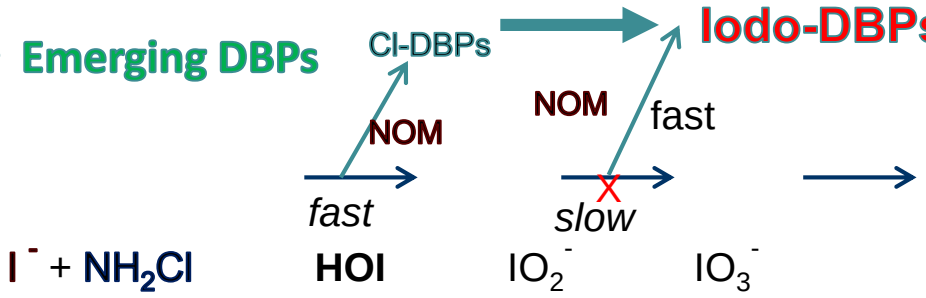
Disinfection By-Products (DBPs)



- > 600 DBPs identified *(Richardson, 2002)*.
- Risk of health effects: bladder/colon cancer, reproductive and developmental effects.
- 50% of the total halogenated material formed in chlorinated water is still unknown.

- **Emerging DBPs**



- Toxicity: iodo- > bromo- > chloro- DBPs

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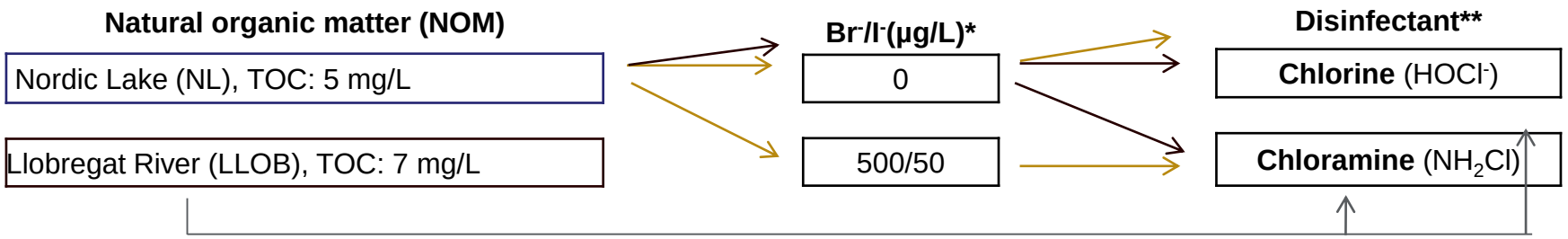
Emerging DBP studies

- To generate DBP mixtures after chlorination and chloramination of different types of water in terms of NOM, iodide and bromide contents.
- To characterize iodo-DBPs in the generated DBP mixtures by means of high resolution mass spectrometry with the Q Exactive GC.

Lab-scale chlorination and chloramination reactions



*Bromide and iodide were added as KBr and KI, respectively.
**[Cl_2]= 4 mg/L for NL, 7.5 mg/L for LLOB, after chlorine demand test.

Blanks: NL water, and LLOB water with no disinfectant added

Reaction conditions:
- **room T^0**
- pH = **7.5** (phosphate buffer)
- stirring for **72 h**
- in the **dark**
- volume = **17 L**

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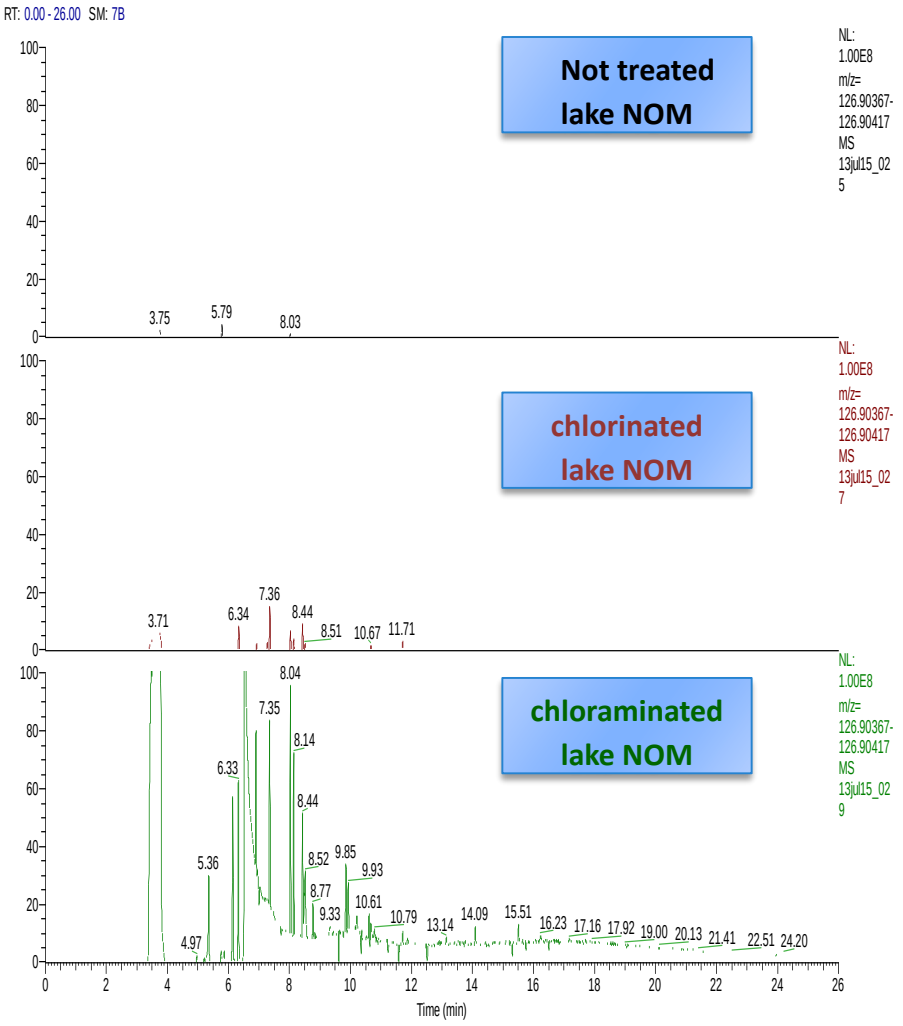
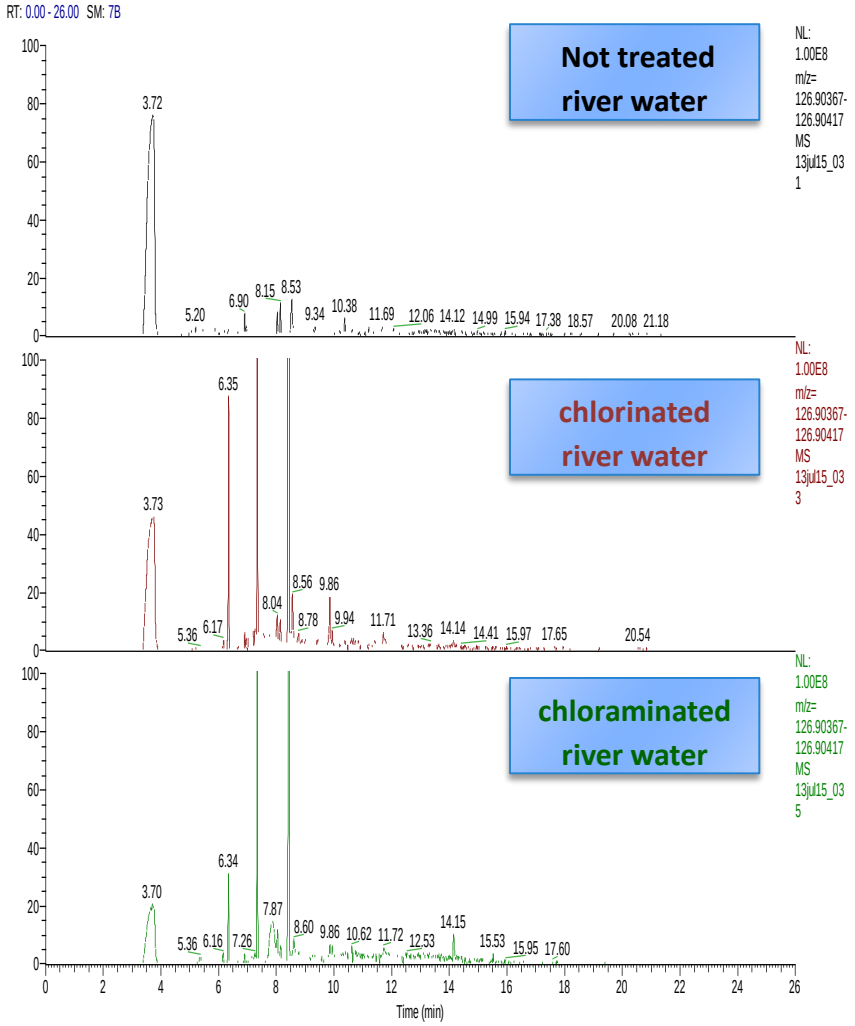
Chromatography (XIC *m/z* 126.90392)





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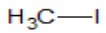
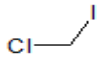
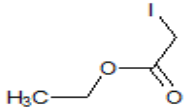
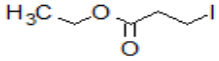
DBPs detected and confirmed in the samples analysed

RT (min)	Identity	Elemental Composition	Chemical Structure	Theoretical m/z (EI)	Measured m/z (EI)	Δ(ppm)	Theoretical m/z $[M+H]^+$	Measured m/z $[M+H]^+$	Δ(ppm)
3.71	Iodomethane	CH_3I		141.92739	141.92745	0.4	142.93522	142.93522	0.0
5.36	Chloroiodomethane	CH_2ClI		175.88842	175.88839	0.2	176.89625	176.89620	0.3
5.76	Iodoacetaldehyde	C_2H_3IO		169.92231	169.92234	0.2	170.93013	170.93014	0.06
7.36	Diiodomethane	CH_2I_2		267.82404	267.82424	0.8	268.83186	268.83192	0.2
8.03	Ethyl iodoacetate	$C_4H_7IO_2$		213.94852	213.94840	0.6	214.95635	214.95627	0.4
8.14	ethyl β-iodopropionate	$C_5H_9IO_2$		n.d.	n.d.	-	228.97200	228.97198	0.07
8.77	Chlorodiiodomethane	$CHClI_2$		301.78507	301.78509	0.1	301.78507	301.78511	0.1
9.85	Bromodiiodomethane	$CHBrI_2$		345.73455	345.73459	0.1	345.73455	345.73446	0.3

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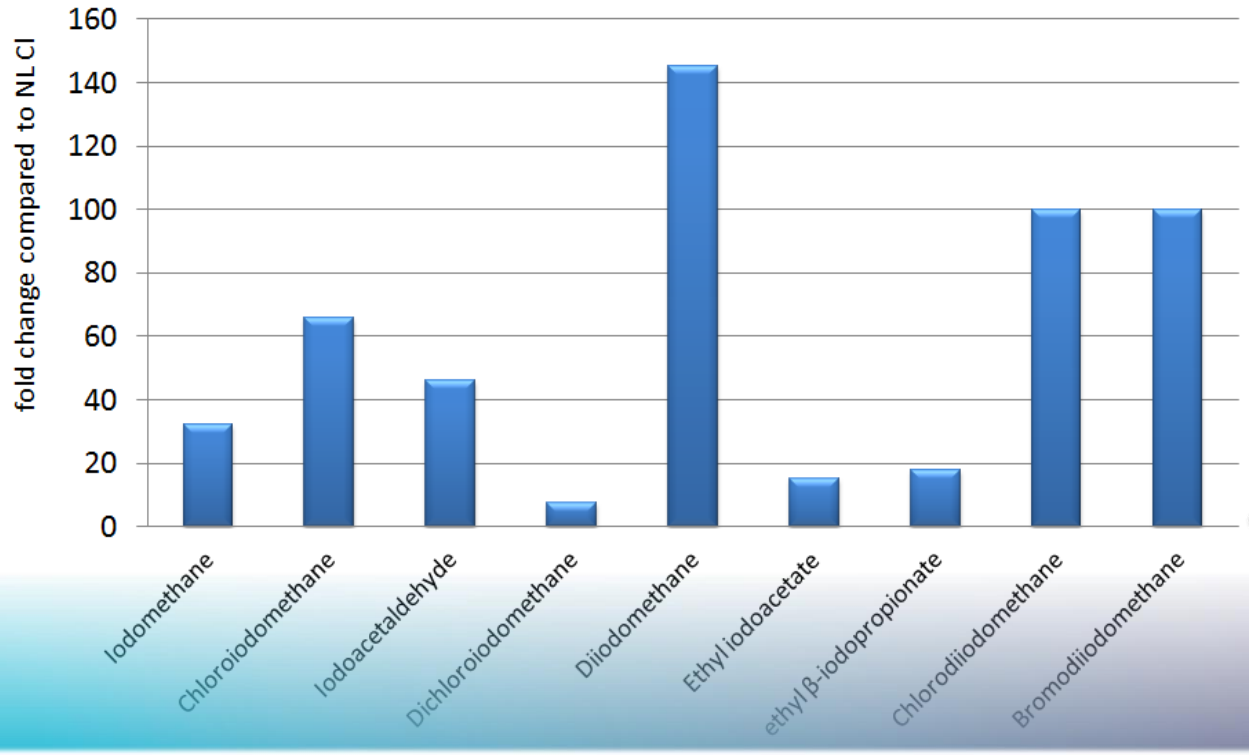
Fold change of DBP's in Nordic Lake water using NH_2Cl vs. Cl



Thermo Scientific Q Exactive GC
Hybrid Quadrupole-Orbitrap GC-MS/MS System

- Hugely powerful HR/AM performance for GC-MS
- Uncompromised quantitative and qualitative capability
- Reliable, robust and easy to operate

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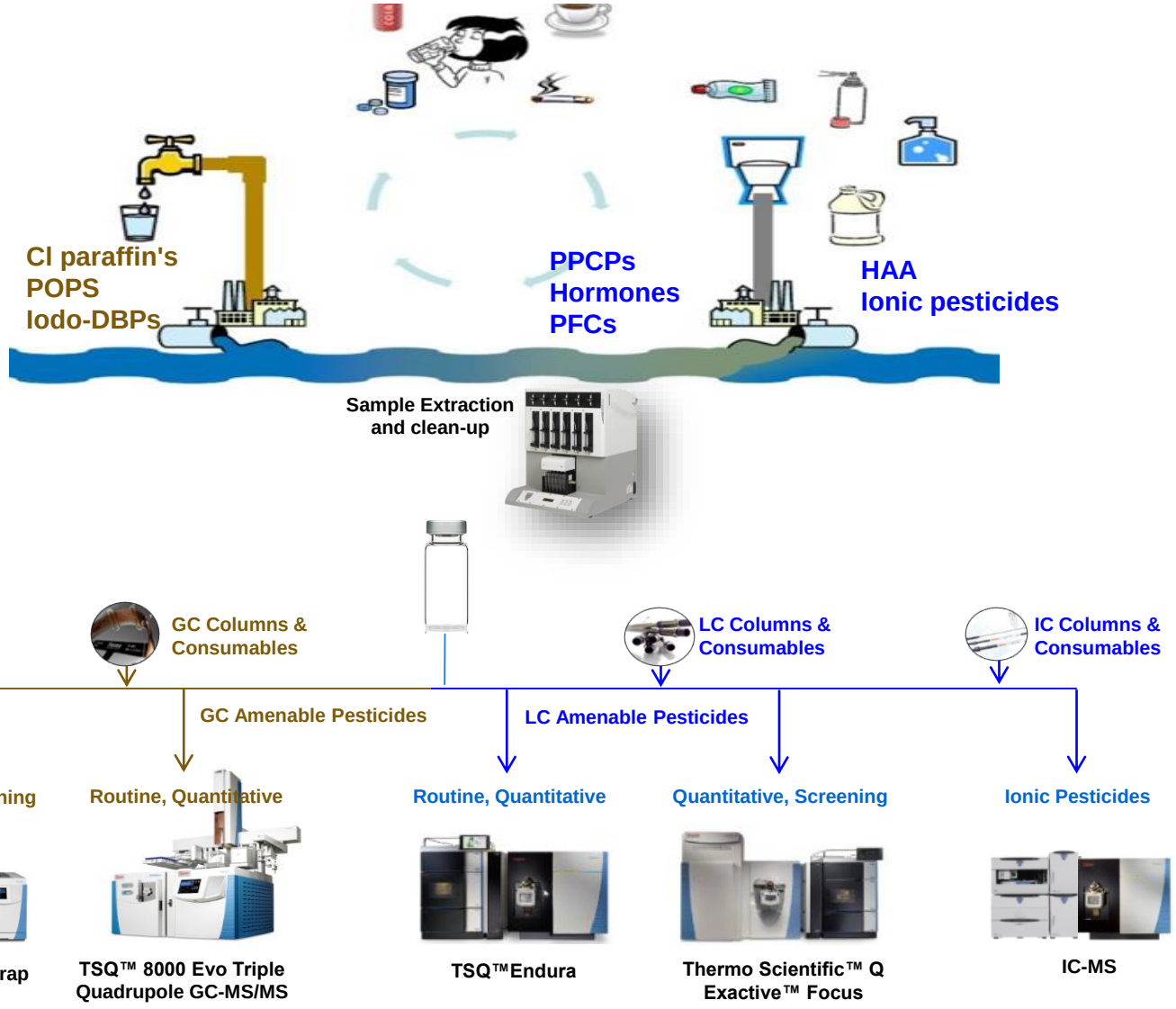
What's your organic contaminant workflow?



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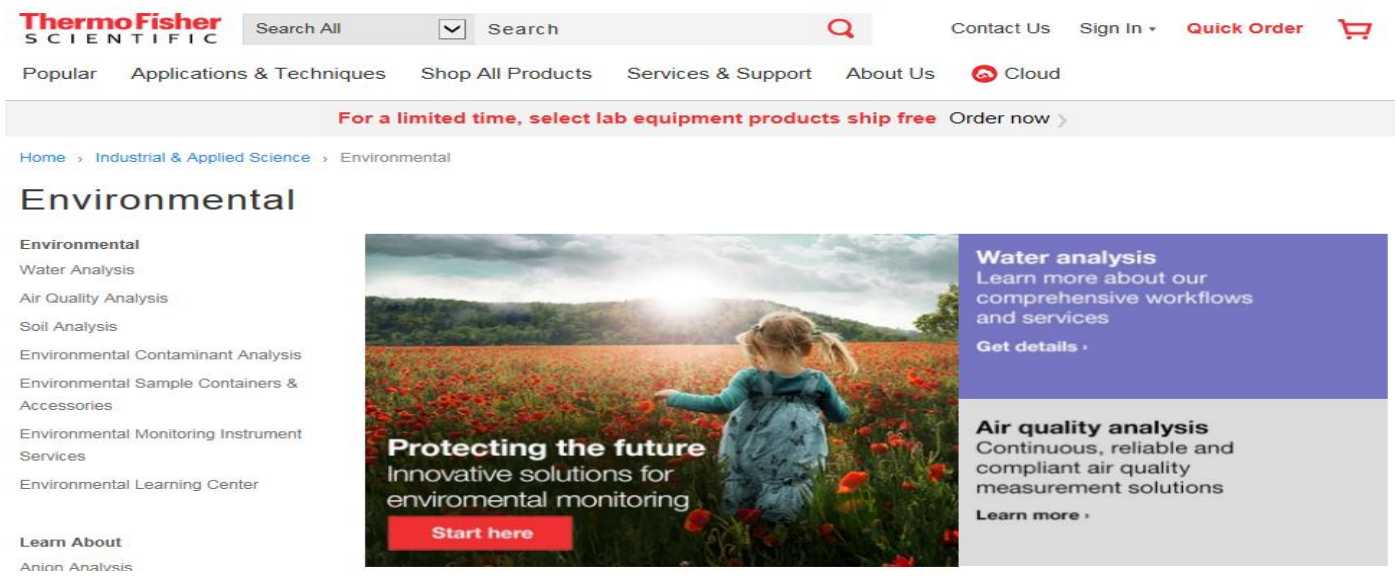
More information ? Visit our website!



Air Analysis

Water Analysis

Soil Analysis

Environmental Contaminant Analysis

- *Inorganic Ions and disinfection Byproducts
- *Metal Contaminants
- *Organic Contaminants
- *Emerging Contaminants

Air Quality Analysis information

Water Quality Analysis Information

- *Water Regulations
- *Analysis of Drinking Water Contaminants (NEW)
- *Wastewater Testing (NEW)
- *Hydraulic Fracturing

Soil Contaminant Analysis

Contaminant Analysis Information

- *Anion Analysis (Multiple NEW pages)
- *Cation Analysis
- *Metal Analysis (Multiple NEW pages)

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- Unique customer value proposition
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Identifying Contaminants in Water

Dr. P. Lee Ferguson

Assoc. Prof. of Civil and Environmental Engineering

Duke University

"Analyzing water for known and unknown pharmaceutical residues, personal care products and industrial chemicals demands precision and speed, without sacrificing sensitivity."

extraction

separation

analysis

identification

Screening 7000+ contaminants, including 9 previously unidentified

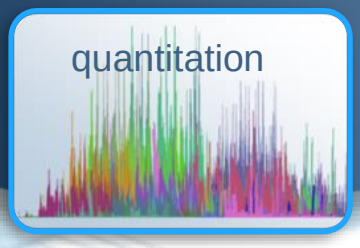
collection

Qualitative

Quantitative

Non-Targeted Analysis

Search for everything



Targeted List Generated

Assay for routine quantitation

Complete solutions, from qualitative to quantitative

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Business Unit / Market Segment Summary Slides

Life Science Mass Spectrometry (LSMS)

Summary:
Mass spectrometry (MS) is an analytical technique that is used for determining the elemental composition of a sample or molecule, and for elucidating the chemical structures of molecules, such as peptides and other chemical compounds. The MS principle consists of ionizing chemical compounds to generate charged molecules or molecule fragments and measuring their mass-to-charge ratios.

Technology / Technique:

- Ion Trap MS
- Single Quadrupole MS
- Triple Quadrupole MS
- Orbitrap MS

Industries, Markets & Applications:

- **Biotech:** Proteomics(i.e. protein discovery, peptide sequencing, biomarker ID), Metabolomics
- **Academic Research:** Proteomics, Metabolomics, Natural Products
- **Government:** Food safety, Environmental, Toxicology, Proteomics
- **Pharmaceutical:** R&D, Pharmacokinetics, Metabolism, Drug Discovery (i.e. verification of chemical synthesis products, target binding, purity, diffusion, kinetic characteristics)
- **Environmental:** Contaminants in water, soil
- **Food & Beverage:** Contaminants in food, beverages
- **Forensics:** drug testing, toxicology screening

Thermo Scientific Model Names:

- Fusion
- Endura
- Quantiva
- Q-Exactive
- FAIMS
- LCQ Fleet
- LTQ Orbitrap Discovery
- LTQ Orbitrap XL
- LTQ Orbitrap Velos
- LTQ FT Ultra
- LTQ Velos
- LTQ XL
- Quantum Access Max
- Quantum Ultra
- Quantum Ultra EMR
- TSQ Vantage
- E Quan Max

Inorganic Mass Spectrometry (IOMS)

Summary:

Inorganic mass spectrometers find their applications in all fields of environmental analysis, geology, geochemistry and material science. They market themselves based on most recent developments in physics and technology for high end research in their particular markets. Academia and industry customers equally swear by the unsurpassed possibilities that this technology provides.

Technologies / Techniques:

- **Magnetic sector mass spectrometers (MS)**
  - Static multi collector MS
  - Scanning double focusing MS
- **Quadrupole MS**
- **Optical absorption spectroscopy**

Industry / Market / Application:

- **Environmental** - Climate research, heavy metal quantification and speciation, Dioxin Analysis
- **Geology** - Geochemistry and geochronology, ultimate precision to elucidate geological processes for exploration and better understanding of earth evolution
- **Food & Forensic** - Authenticity control, export / import regulations, food safety
- **Material Science** - Manufacturing and quality control for sophisticated materials such as super alloys, silicon for semicon and solar cell industry
- **Nuclear** – Enrichment control for fuel rods; production and proliferation control

Thermo Scientific Model Names:

- Delta Ray
- Element GD
- Element2
- Element XR
- X Series 2
- Delta V advantage
- Delta V plus
- MAT 253
- DFS
- Triton
- Neptune
- Argus
- Helix SFT
- Helix MC
- Uranus

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Ion Chromatography (IC)

Summary:
Ion Chromatography is an instrumental technique for separating and measuring substances that are dissolved in water. IC separations are done using one of 3 mechanisms: ion exchange (>90% of market), ion exclusion, ion pairing.

Technology / Technique:

- **IC:** Ion Chromatography
- **RFIC:** Reagent Free Ion Chromatography, No handling acids or bases – Just Add Water!
- **Suppression**: Chemically transforms column effluent, increases response of analytes + reduces background signal from eluent

Industries, Markets & Applications:

- **Environmental Testing Labs:** Anions & Cations in Drinking, Waste Water, Soil & Air
- **Water providers & Wastewater treatment facilities:** Anions & Cations in Drinking, Waste Water, Soil & Air
- **Pharmaceutical companies:** Ionic impurities
- **Chemical/petrochemical companies:** Ionic impurities
- **Food producers and processors:** Nutrients
- **Power utilities:** Chloride and Sulfate in Biofuels
- **Electronics manufacturers:** Ionic Impurities in High Purity Water
- **Mining/metals/plating companies:** Ionic impurities

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Sample Preparation

Summary:

Sample preparation instruments help take samples from solids and prepare them typically for later workflow steps involving chromatography. The instruments provide higher and more repeatable throughput relative to manual processes.

Technology / Technique:

- **ASE:** Accelerated solvent extraction
- **SPE:** Solid phase extraction

Industries, Markets & Applications:

- **Environmental Testing Labs:** Anions & Cations in Soil
- **Pharmaceutical companies:** Ionic impurities
- **Food producers and processors:** Nutrients
- **Mining/metals/plating companies:** Ionic impurities

Thermo Scientific Model Names:

- ASE™ 350 Accelerated Solvent Extractor
- AutoTrace™ 280 Solid-Phase Extraction

Liquid Chromatography (LC)

Summary:
Liquid chromatography enables the physical separation, quantification, and identification of complex substances across multiple industries. Scientists use this technology to develop new drug compounds, verify results in QA/QC, and identify unknown contaminants in various products. Our chromatographic systems increase laboratory productivity by integrating high throughput technologies with dedicated separation and detection solutions.

Technology / Technique:

- **HPLC:** High Performance Liquid Chromatography
- **UHPLC:** Ultra High Pressure Liquid Chromatography
- **Nano-LC:** Nano Liquid Chromatography
- **Multiplexing:** Parallel Liquid Chromatography
- **LC/MS:** Liquid Chromatography Mass Spectrometry
- **Chromatography Data System**: Software

Industries, Markets & Applications:

- **Pharmaceutical:** drug development and quality control
- **Forensics/Toxicology:** separation of unknown mixtures
- **Environmental:** water and soil analysis
- **Clinical:** separation of biological substances
- **Food & Beverage:** R&D of new products and quality control
- **Academia:** research and education
- **Food Safety:** identification of unknown contaminants

Thermo Scientific Model Names:

- EASY-nLC II
- Transcend II Systems
- MSQ Plus
- Spectra System
- Ultimate 3000
- Chromeleon Data System Software

Gas chromatography (GC, GC/MS)

Summary:
Gas chromatography (GC) and gas chromatography/mass spectrometry (GC/MS) combines separation with the today most advanced detector types used to identify and quantify substances in a prepared sample. GC and GC-MS systems are powerful tools used in markets and application areas for routine analysis of drug detection, food and water contamination, air quality etc. as well as in research and academia.

Technology / Technique:

- GC, GC/MS, GC/MSMS

Industries, Markets & Applications:

- **Environmental:** Air, Water & Soil quality
- **Food Safety:** Pesticides, POPs
- **Forensics, Toxicology:** THC in oral fluids, Alcohol in blood…
- **Petrochemical:** DRO, GRO, Biofuels

Thermo Scientific Model Names:

- Trace 1300
- FOCUS
- TRACE
- DSQ II
- ISQ
- ITQ
- TSQ Quantum XLS
- AS3000
- TriPlus
- QuanLab Forms
- ToxLab Forms
- EnviroLab Forms
- ChromQuest
- Chrom Card
- Microstructure

Trace Elemental Analysis (TEA): AA/ICP/ICPMS

Summary:

Range of advanced analytical instrumentation used to detect elements in trace quantities down to below 1 part per trillion (ppt).

Technology / Technique:

- **AA – Atomic Absorption:** longest established trace elemental technique, which is single element technique.
- **ICP – Inductively Coupled Plasma Optical Emission Spectrometry**: known for routine, rugged analysis technique of choice for many elemental analysis applications from percent to sub-ppb levels
- **ICP-MS - Inductively Coupled Plasma Mass Spectrometry:** most sensitive elemental analysis technique with sub-ppt detection capability, and is typically applied to cleaner matrix samples.

Target Industries / Applications:

- Quality Control & Regulatory Compliance of elemental content
  - **Environmental:** Drinking water
  - **Food safety**
  - **Petrochemical**
  - **Pharmaceutical**
  - **Metallurgy**
  - **Chemistry / Research**

Thermo Scientific Model Names:

- iCap Q
- Element 2 / GD
- iCAP 7000 series
- iCE 3000 series
- iCE 3400/3500 iCEAA
- X Series 2

Trace Elemental Analysis (TEA): OEA(FLASH)

Summary:

Organic Elemental Analysis is a technique for analyzing any micro (mg) samples by combustion for the elements C,H,N,O, S (FLASH 2000). Virtually any type of material can be analyzed by this technique, and so it is found in many applications: materials (plastic, glass, ceramic, rubber etc), oils, food, geological and forensic. The same analyzer can be used as a hyphenated technique to couple to and IRMS (Isotopic Ratio Mass Spectrometer) which is a very sensitive technique used in geological and food authenticity applications. Macro samples (up to 2gm) can also be monitored for a specific analysis to determine N-Protein, primarily in food (FLASH 4000).

Technology / Technique:

- **OEA (FLASH):** Organic Elemental Analysis

Target Industries / Applications:

- **Food Safety**
- **Materials Analysis:** Plastics, Ceramics, Rubbers

Thermo Scientific Model Names:

- FLASH 2000
- FLASH 4000

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