Research Project:
Non-target and Suspect Screening of Contaminants of Emerging Concern in lower Columbia River

Columbia River Basin Restoration Program (CRBRP) Grant Program
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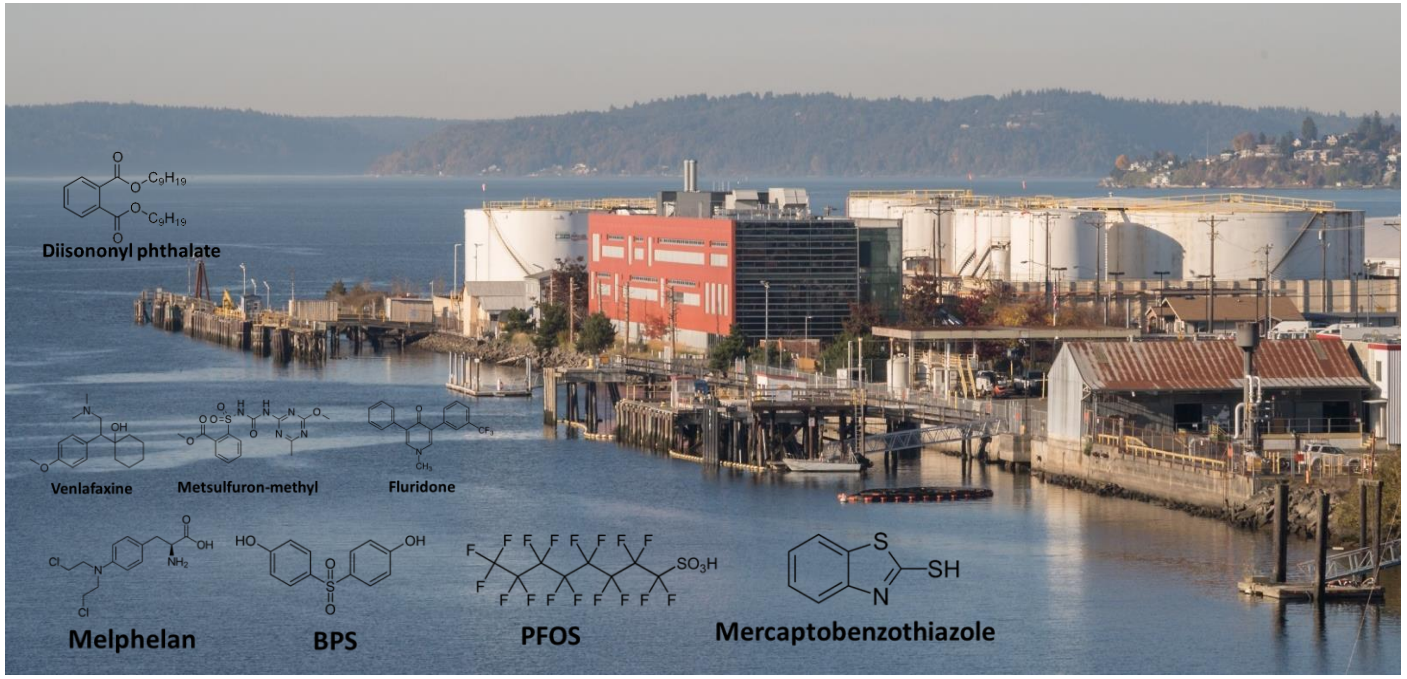
Project:

Characterize the occurrence of Contaminants of Emerging Concern in the Lower Columbia River using High Resolution Mass Spectrometry methods

Utilize multiple measures of biological impacts to understand their potential for harm



Tian et al, ES&T, 2019

Motivation:

- CECs are in the environment. Some have been associated with environmental harm.
  - Endocrine disruption, reduced survival, pre-spawn mortality syndrome
- Improving our understanding of CECs is a priority of ecosystem recovery programs

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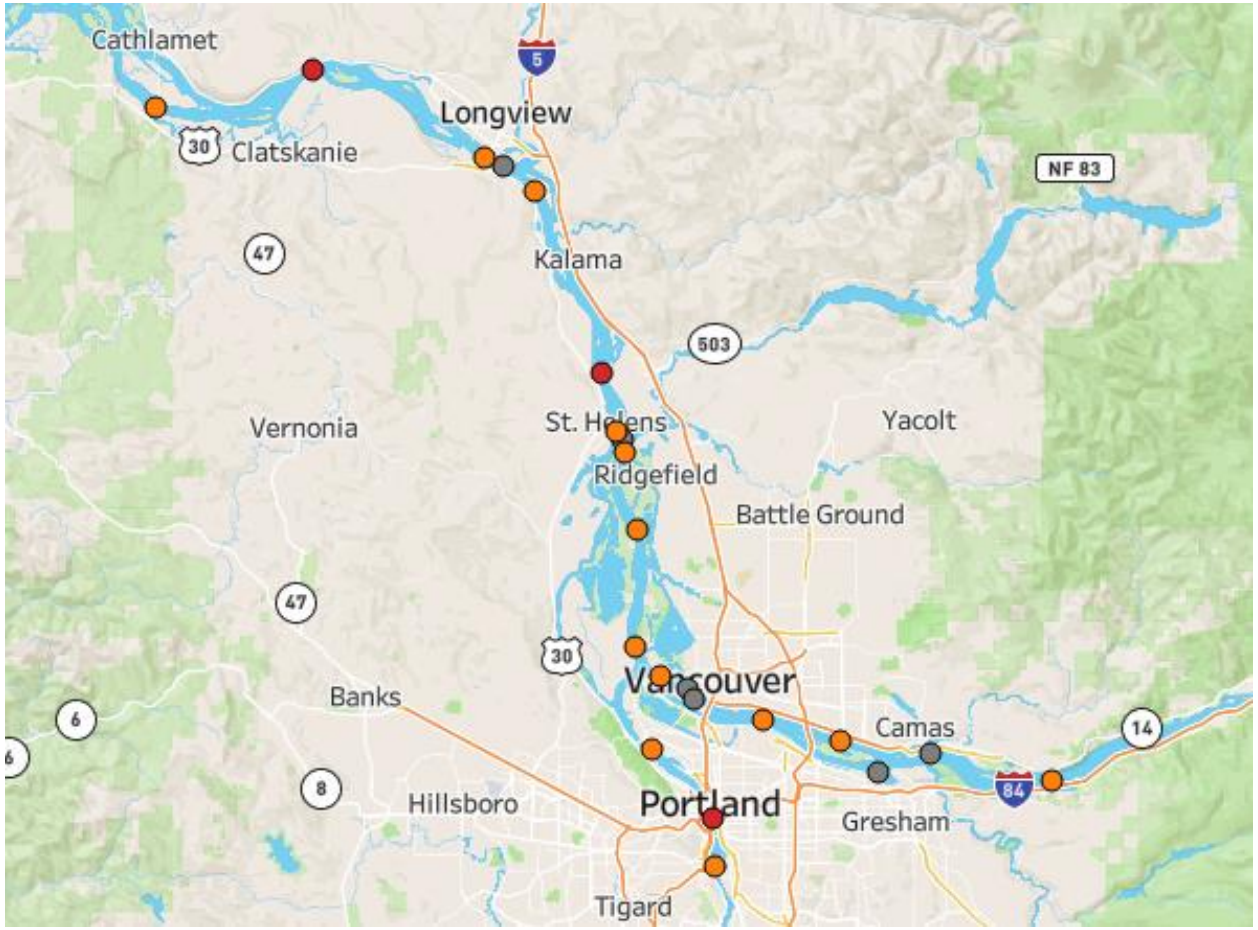
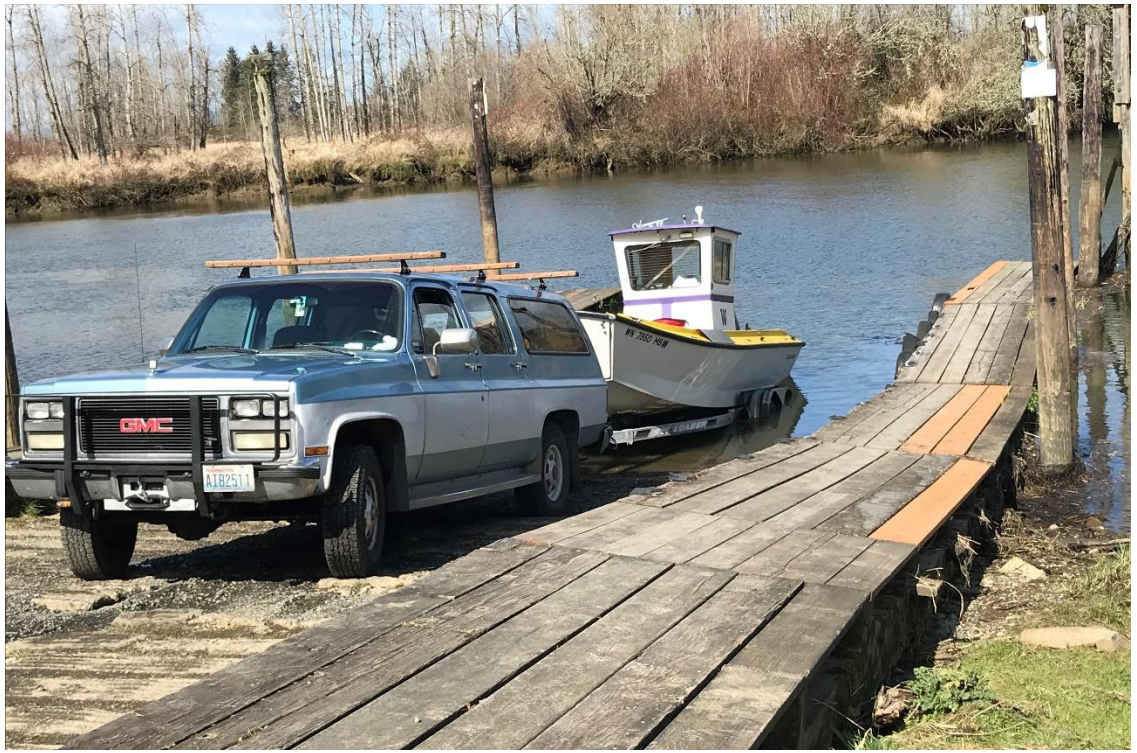
Monitoring



- 16 sampling locations
  Selected in consultation with USGS Oregon Water Science Center in order to characterize potential areas of impact based on past monitoring or inputs
- Four sampling events
  Two – February and March
  Two – August and September

Note: Selected WWTP outfall locations are shown for reference only. WWTP effluent will not be sampled under this project.

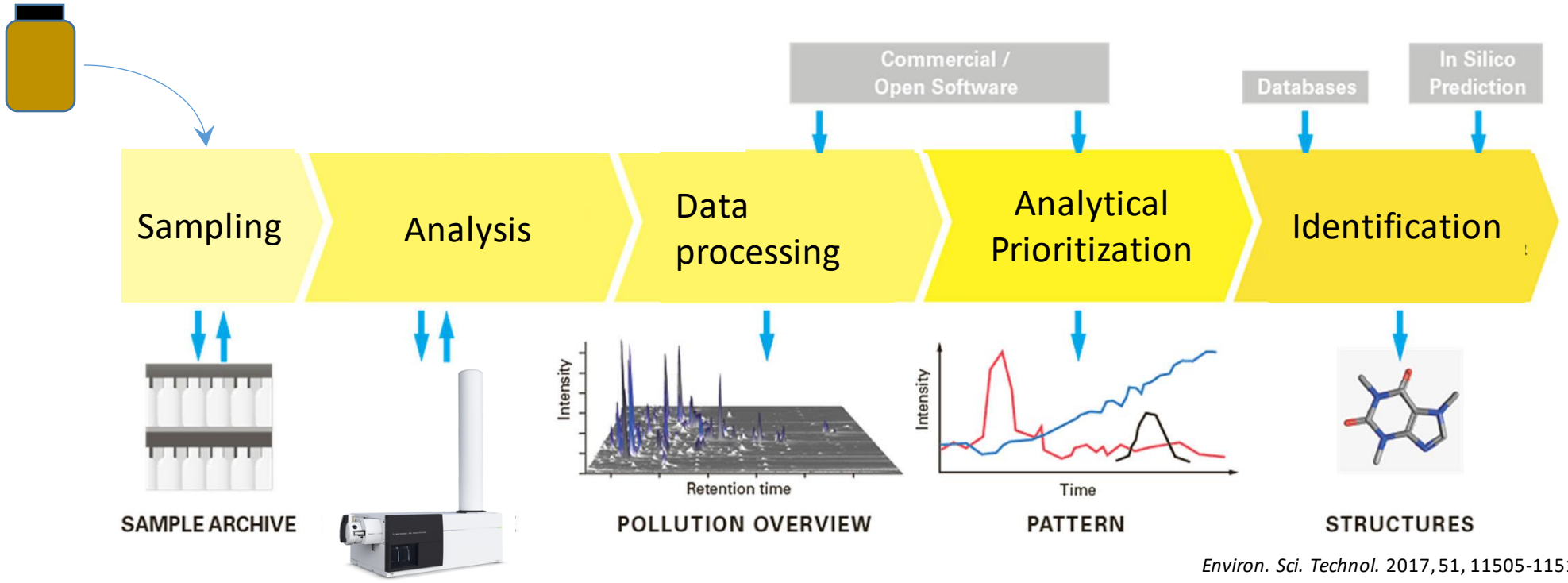
Columbia River Sampling



Analysis

Non-target screening based on high resolution mass spectrometry

- Detect 100s-1000s of unique compounds in a given sample without a priori knowledge of compound IDs
- Analytical prioritization based on replication and occurrence patterns

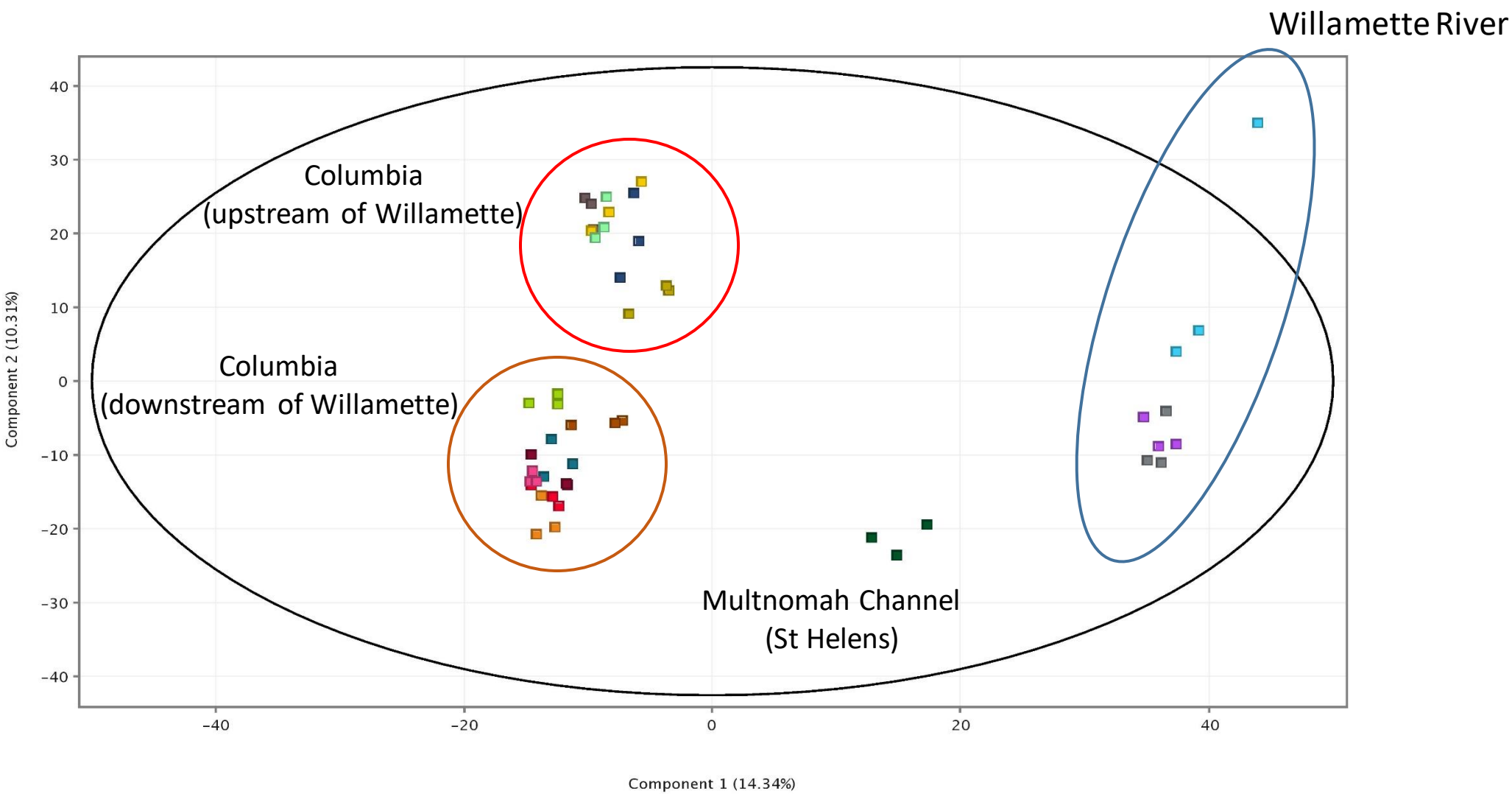


Environ. Sci. Technol. 2017, 51, 11505-11512 (with modification)

Data Analysis

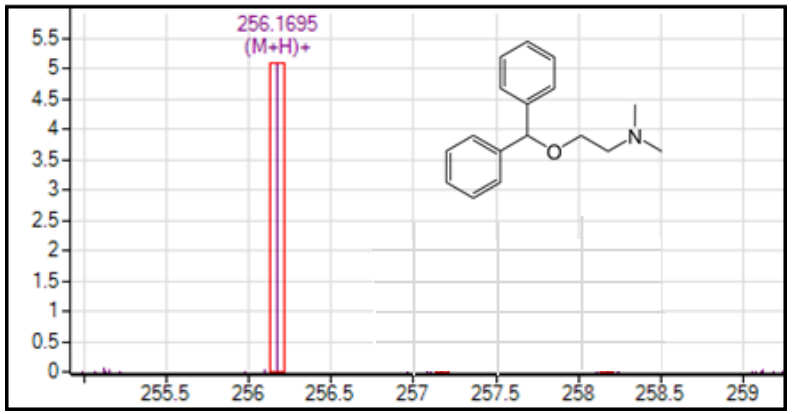
- System wide based on broad comparative analysis

- Compound focus
  - Identify based on in house database of > 1000 compounds. Pharmaceuticals, automobile related compounds, common use chemicals, agricultural antibiotics, etc.
  - Identify compounds based on existing libraries and fragmentation patterns
  - Identify potential source contributions based on existing source signature patterns


Willamette River
Columbia
(upstream of Willamette)
Columbia
(downstream of Willamette)
Multnomah Channel
(St Helens)
Component 2 (10.31%)
Component 1 (14.34%)
40
30
20
10
0
-10
-20
-30
-40
-40
-20
0
20
40

HRMS Data – fragmentation (MS/MS)

Diphenhydramine



MS only

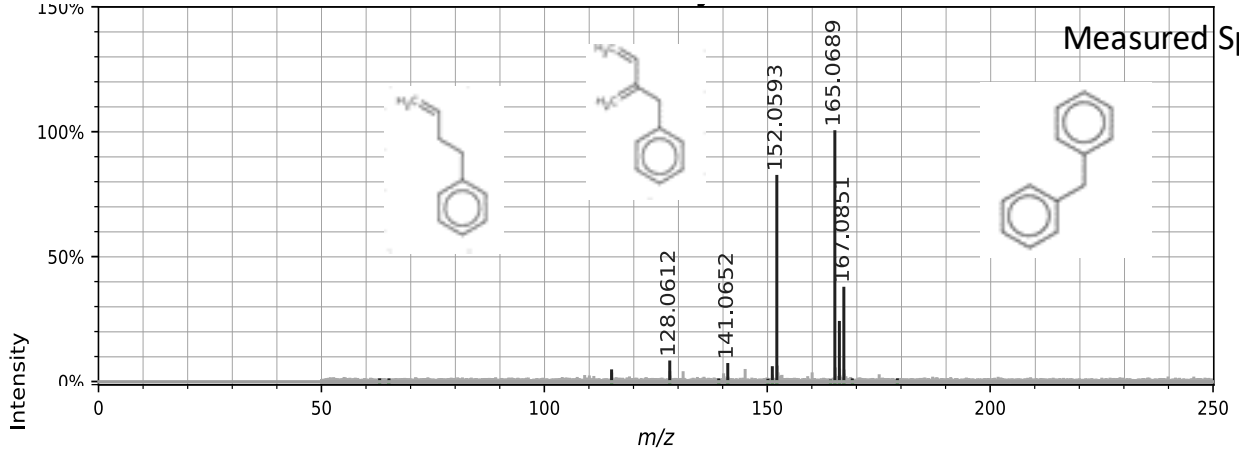
Accurate Mass of Compound

$C_{17}H_{21}NO$

(Five Compounds with Same Formula)

MSMS

Increase Confidence of Identification

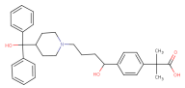


Library Spectra

Tris(2-chloroisopropyl) phosphate
Tris(2-butoxyethyl) phosphate

- Replacement flame retardant used in foams
- Present in house dust and WWTP effluent
- Evidence of bioactivity (ToxCast) and endocrine disruption (Liu et al., 2016)
- TBOEP exposure of zebrafish decreases the average number of egg production, as well as hatching success and survival rates in offspring (Xu et al., 2017)

Fexofenadine



- Antihistamine
- Evidence of bioactivity
- Evidence of bioconcentration and behavioral change in aquatic insects (Josson et al., 2014)

Acetyl Tributyl Citrate

- Replacement plasticizer for phthalates
- Evidence of bioactivity
- Evidence of endocrine disrupting activity (Park et al., 2017)

Prioritization

Effects data and threshold

Two different data sets to identify ecological thresholds that are indicative of a biological response. Lower threshold → potentially more important compound

- Predicted No Effects Concentration (PNEC) from EU NORMAN program results
- CompTox – results of laboratory testing from Tox21 and ToxCast programs includes information on interactions with or effects on cells, proteins, DNA, RNA, receptors

Outcome

- Improved characterization of the occurrence of trace organic contaminants (CECs) in the lower Columbia River
- Screening level evaluation of potential impacts of presence of CECs
- Identification of priority contaminants and (potentially) sources

Thank You

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