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

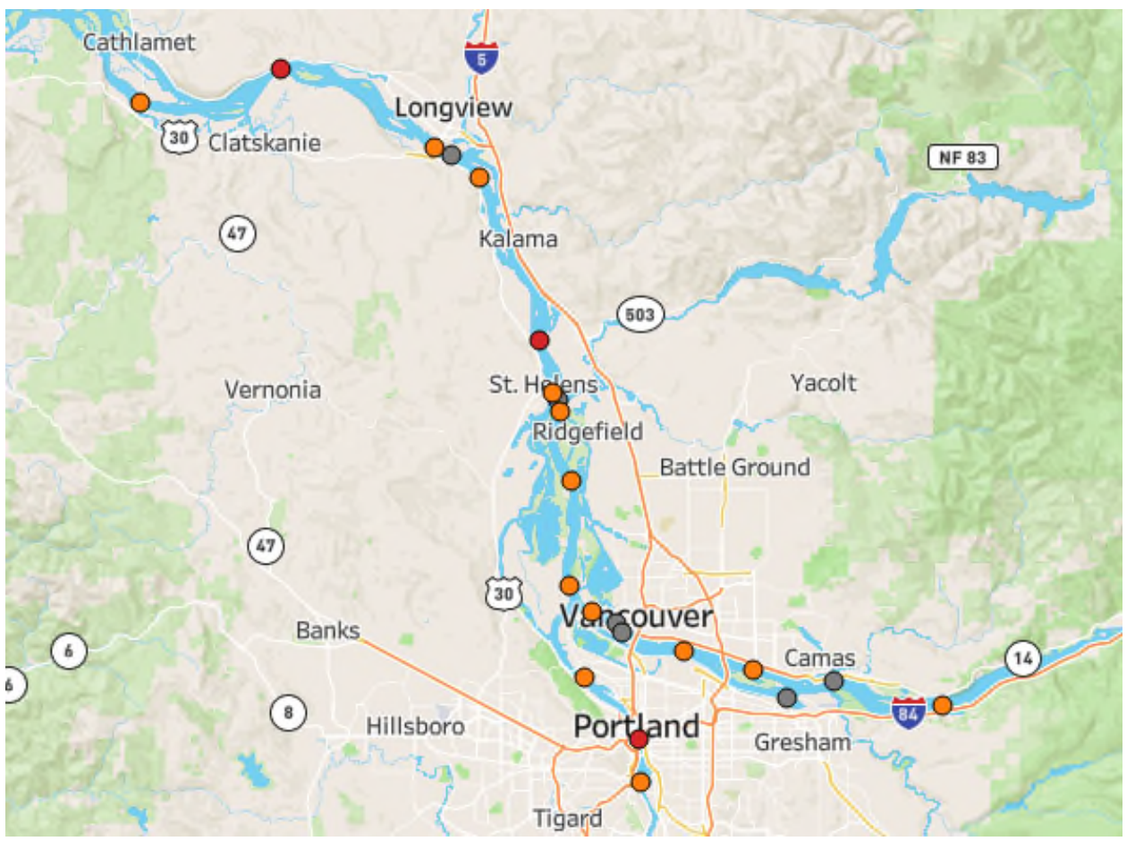
Utilize multiple measures of biological impacts to understand their potential for harm

Tian et al, ES&T, 2019

Motivation:

- Exposure to some CECs have been associated with ecosystem health impacts
  - Endocrine disruption, reduced survival, pre-spawn mortality syndrome
- Improving our understanding of CECs is a priority of ecosystem recovery programs

Monitoring



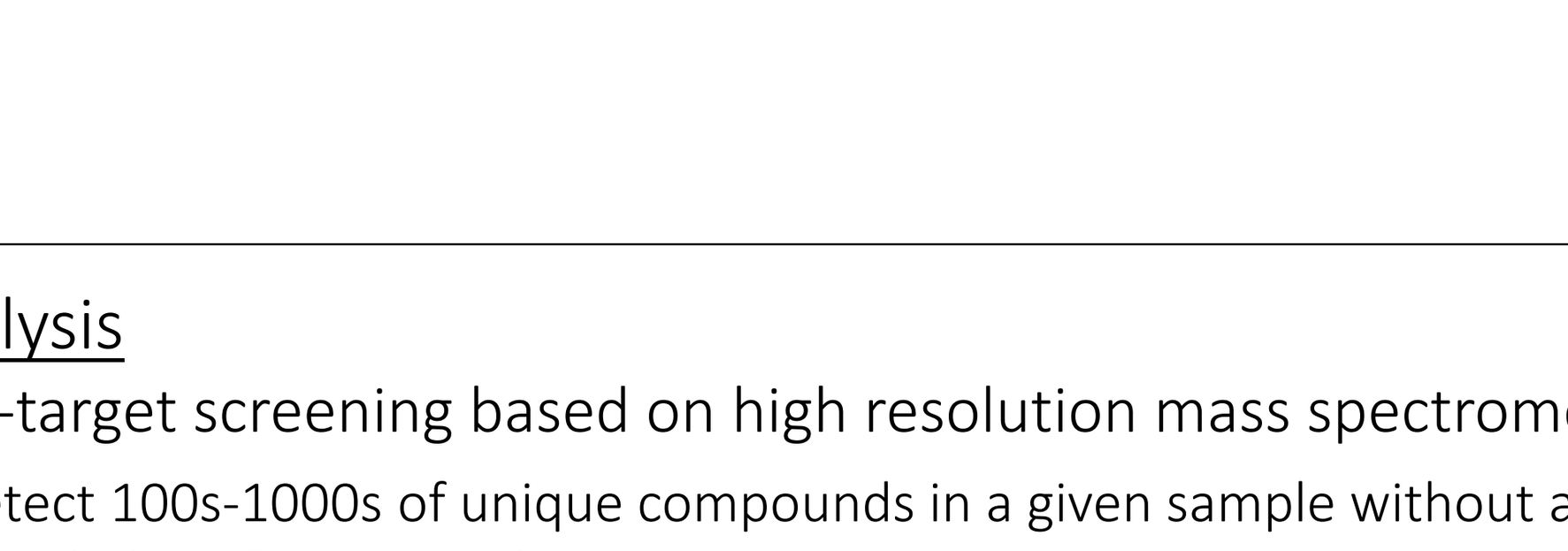
- 15 sampling locations
  Selected in consultation with USGS Oregon Water Science Center in order to characterize potential areas of impact based on past monitoring or inputs
- Four sampling events
  Two – February and March
  Two – August and September

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

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)

Analysis

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

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Prioritization

Challenge –
there are limited ecotoxicological studies/information for many of the compounds we are identifying

Response –
Chemical Screening.
Compare levels of occurrence with potential effects levels in order to identify those that are of potential concern

Performing in conjunction with Puget Sound Ecosystem Monitoring Program toxics workgroup project
(Ruth Sofield WWU and Andy James UW Tacoma)

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Prioritization

Effects data and threshold

- 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

$$\frac{Environmental\ Concentration}{Effects\ Level} = Toxicity\ or\ Effects\ Ratio$$

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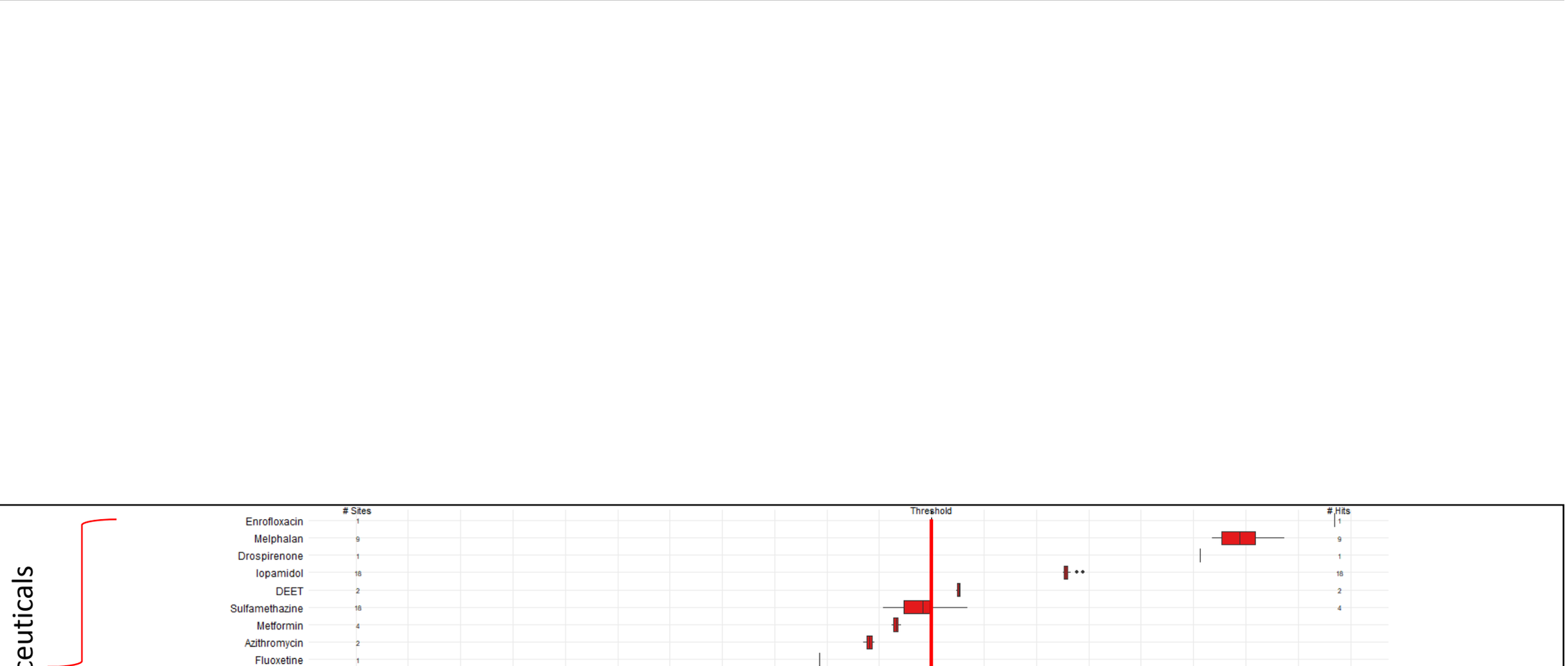

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Outcome

- 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 potential sources

Thank You

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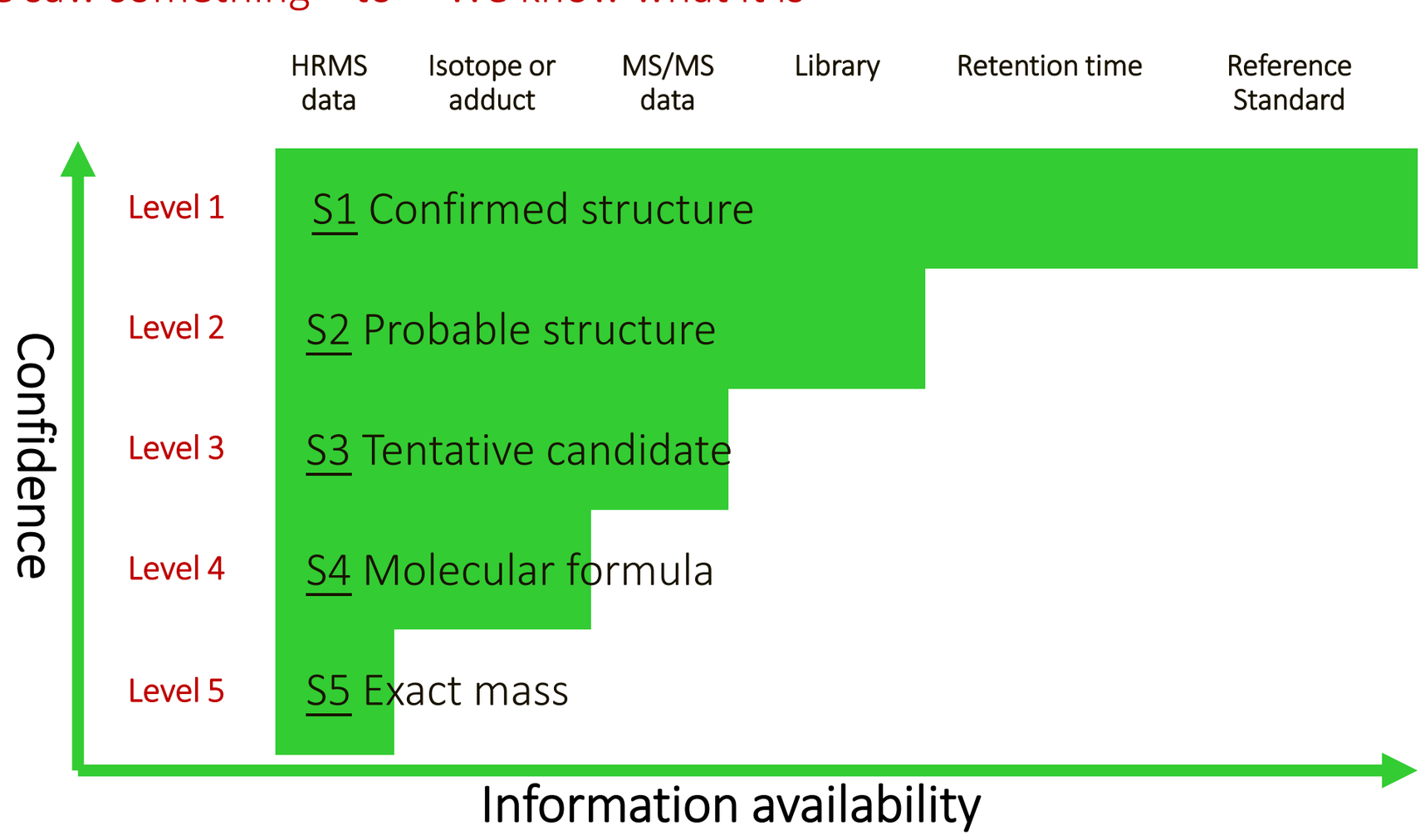
Confidence level in HRMS detections

"We saw something" to "We know what it is"



Schymanski et al., 2014 ES&T

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Suspect and non-target screening workflow

- In-house PCDL with exact mass and retention time (~1100)
- NORMAN PCDL for extensive suspect screening (~37,000, mass only)
- Batch mode *in silico* fragmentation

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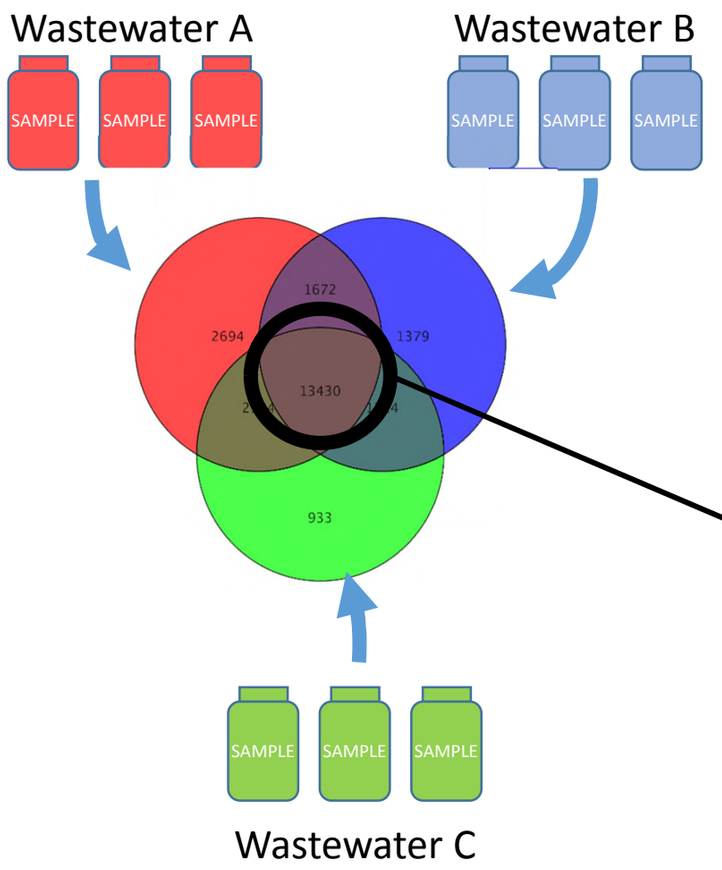
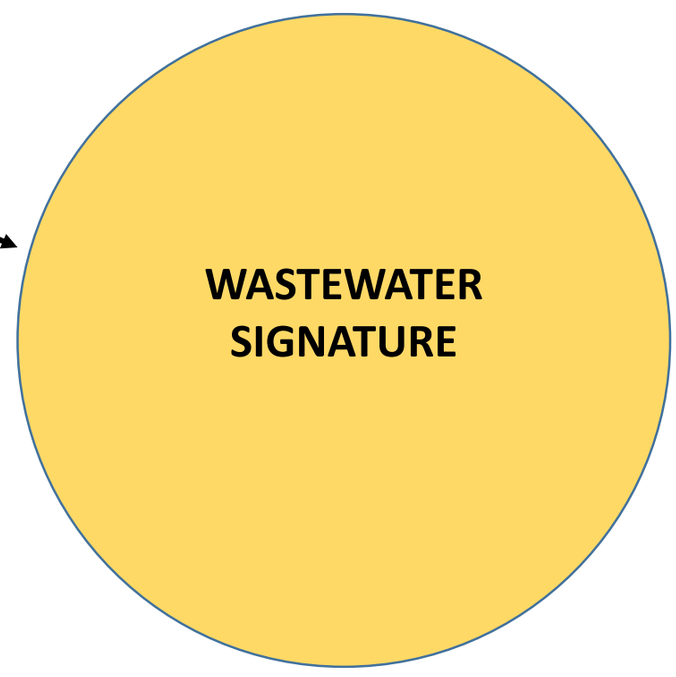


Signature Development

- Identify chemicals that are present in multiple replicates for multiple events (minus process blanks)



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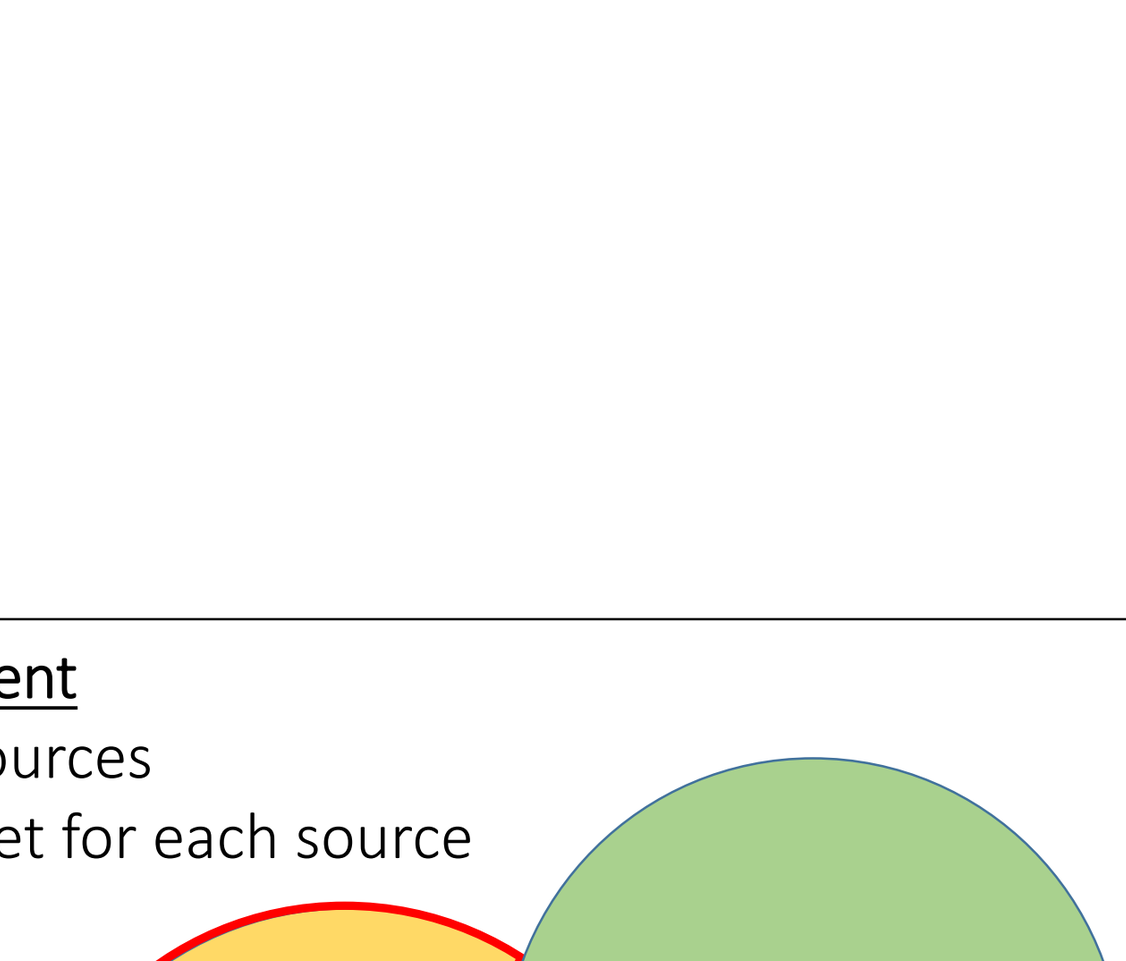
Signature Development

- Add additional sources
- Identify unique set for each source



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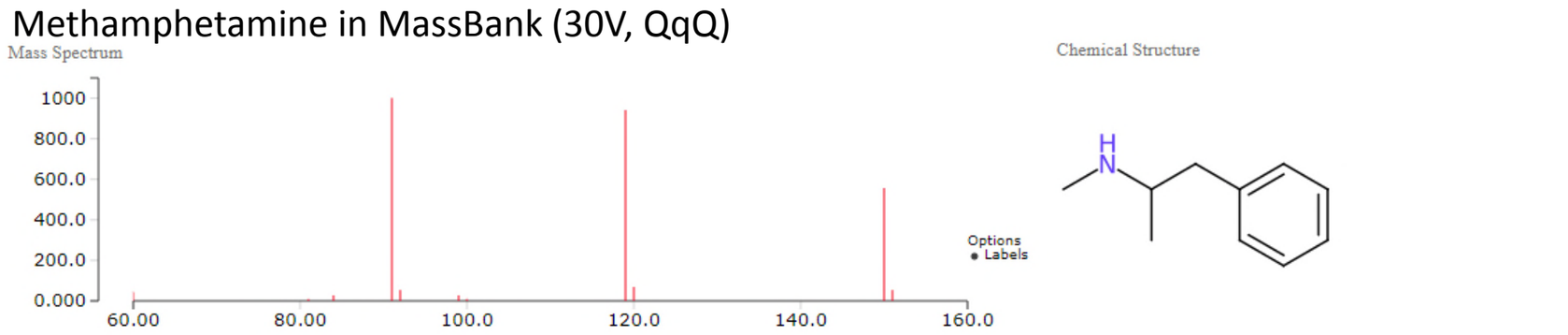
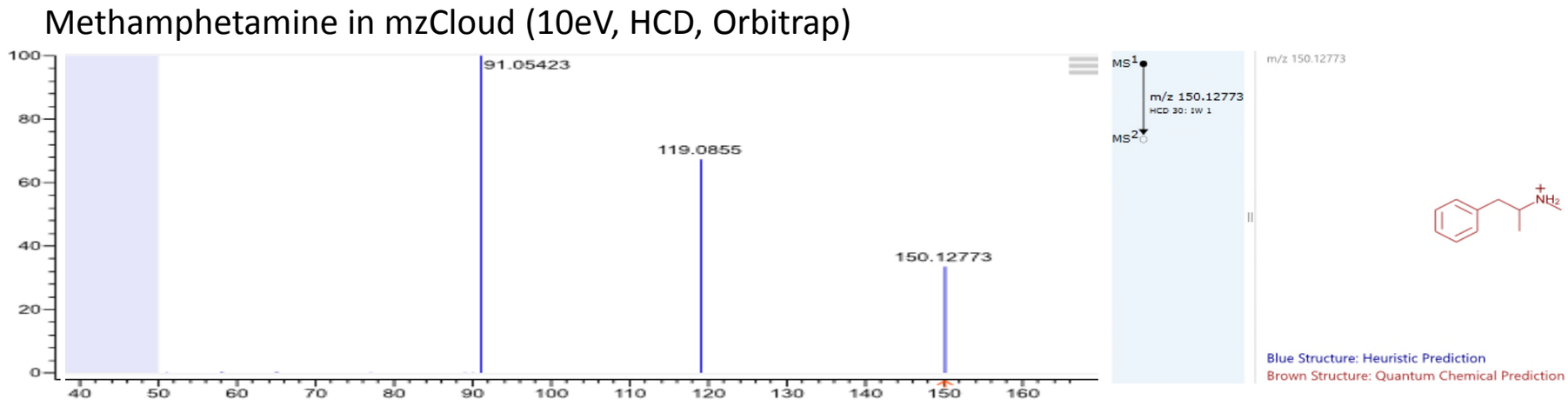
Methamphetamine MSMS in spectral libraries

Methamphetamine in MassBank (30V, QqQ)



Methamphetamine in mzCloud (10eV, HCD, Orbitrap)



https://massbank.eu/MassBank/RecordDisplay.jsp?id=WA000856&dsn=Waters

https://www.mzcloud.org/DataViewer#/Main/reference$1835/T5559%23Standard/Recalibrated/647078