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Flame Retardants in Ten Washington State Waterbodies

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This addendum is an addition to an original Quality Assurance Project Plan. It is not a correction (errata) to the original plan.

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Addendum to Quality Assurance Project Plan

Flame Retardants in Ten Washington State Waterbodies

February 2018

Approved by

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Signatures are not available on the Internet version.
EAP: Environmental Assessment Program

3.0 Background

3.1 Introduction and problem statement

Persistent, bioaccumulative, and toxic chemicals (PBTs) are a broad group of chemical compounds that are persistent in aquatic systems, build up in aquatic food webs, and cause harm to wildlife or humans. PBTs include some halogenated flame retardants, per- and poly-fluoroalkyl substances (PFAS), and many other chemical classes. Washington State currently identifies 27 chemicals and chemical groups as PBTs in the state's PBT Rule (WAC 173-333). The State Departments of Ecology (Ecology) and Health (DOH) develop chemical action plans (CAPs) for chemicals from this list to compile information on use and exposure in Washington and recommend actions to protect human health and the environment. Ecology and DOH have developed CAPs for mercury, polybrominated diphenyl ethers (PBDEs), lead, polycyclic aromatic hydrocarbons, and polychlorinated biphenyls. A CAP for PFAS is currently being drafted.

The PBT Rule defines a process to periodically review and update the PBT List and to prioritize the order in which chemicals will be selected for CAP development. Ecology plans to draft an updated PBT List and reprioritize a multi-year schedule for chemicals in the near future. Screening exercises have estimated that hundreds of chemicals currently produced and used have potential PBT properties (Brown and Wania, 2008; Howard and Muir, 2010; Strempel et al., 2012). As Ecology updates the PBT List, it is important that current use PBT chemicals be included for consideration. However, very little environmental information exists on these emerging PBTs. This data gap highlights the need for expanding the range of chemicals to be identified, evaluated, and monitored.

Ecology's PBT Monitoring Program regularly conducts studies to determine environmental levels and trends of chemicals that have been addressed by CAPs. This monitoring program also conducts research into emerging contaminants that may need to be addressed by future CAPs or other agency actions to reduce toxic threats. Ecology is currently carrying out a study in 2017/2018 to quantitatively analyze legacy and current use flame retardants in surface water, sediment, and fish tissue in Washington State waterbodies (original QAPP, Mathieu, 2017).

For this 2017/2018 study, target analytes in freshwater fish tissue collected from three locations include halogenated flame retardants and PBDEs. This QAPP addendum documents an additional component to this project to collect more information on potential halogenated compounds present in fish tissue in these waterbodies. Ecology will send a total of six fillet tissue samples to the laboratory of University of Washington – Tacoma (UWT) Center for Urban Waters (CUW) for non-targeted screening of anthropogenic halogenated compounds by quadrupole time of flight liquid chromatography tandem mass spectrometry (QTOF LC-MS/MS). The non-targeted screening will seek to identify a large range of potential PBT chemicals present in the fish tissue samples. This information will help inform and prioritize target analyte lists in future monitoring studies.

3.2 Study area and surroundings

Freshwater fish samples were collected under the original QAPP (Mathieu, 2017) from Lake Ozette, Lake Spokane, and Lake Washington. Archived fish tissue samples from these locations will be sent to UWT CUW for non-targeted screening. Study area and surroundings were described in the original QAPP.

3.2.2 Summary of previous studies and existing data

The use of non-targeted screening through time of flight mass spectrometry analysis has been increasing in environmental contaminant studies. Targeted analysis of specific analytes, typically used in monitoring programs, uses internal reference standards for identification and quantification of an analyte or analyte group. Because this type of monitoring is limited by budgetary resources, information is gained on only a fraction of chemicals that may be present in the sample. Non-targeted screening through time of flight mass spectrometry instruments can be used to identify what compounds may be present in a sample and the relative abundance of those compounds. This information is helpful for monitoring programs to prioritize targeted analyte suites. Time of flight mass spectrometry studies have successfully identified halogenated chemicals with persistent and bioaccumulative potential in environmental samples (Pena-Abaurrea et al., 2014; Jobst et al., 2013; Hashimoto et al., 2013).

Non-targeted screening studies in Washington have primarily focused on contaminants of emerging concern in the Puget Sound area. Du et al. (2017) describes the development of suspect and non-target screening methods for detecting organic contaminants in highway runoff and fish tissue. In their study, QTOF LC-MS/MS was used to identify high priority compounds that adult coho salmon are exposed to via urban stormwater runoff, such as pharmaceuticals and personal care products. Their screening data indicated that novel or poorly characterized organic contaminants are present in highway runoff and many are detected in exposed fish tissue.

Toxics monitoring programs in other states have adopted non-targeted screening using time-of-flight instruments to help inform their targeted monitoring analyte lists. The North American Great Lakes Fish Monitoring and Surveillance Program (GLFMSP) utilizes QTOF UPLC-MS/MS as a proactive approach in identifying contaminants of concern in Great Lakes predator fish species (Crimmins et al., 2013). Their non-targeted and suspect screening program has identified novel per- and poly-fluoroalkyl substances (PFAS) in trout tissue (Fakouri Baygi et al., 2016; Crimmins et al., 2014). Research done at U.S. EPA's National Exposure Research Laboratory has also identified novel PFAS compounds in environmental samples near manufacturing facilities using time of flight analysis (Strynar et al., 2015).

A non-targeted analytical approach was employed in California monitoring programs to identify halogenated compounds in marine biota (Millow et al., 2015; Shaul et al., 2015). In piscivorous seabird eggs, non-targeted screening identified an average of 111 halogenated organic compounds of which 84 were regularly detected through targeted analysis (Millow et al., 2015). The study identified 27 compounds that were either unmonitored or previously unknown. In bottlenose dolphin blubber sampled off the coast of California, non-targeted screening identified

180 anthropogenic halogenated organic compounds, the majority of which (74%) are not typically monitored for (Shaul et al., 2015).

3.2.3 Parameters of interest and potential sources

The parameters of interest include known and unknown PBT chemicals in freshwater fish tissue. The non-targeted screening will seek to identify compounds in the samples that are anthropogenic halogenated organic compounds and/or compounds identified in existing literature as potential PBTs. PBTs are a priority class of chemicals because of their persistence in the environment, bioaccumulation in wildlife and humans, and toxicity.

Environmental releases of PBTs in the environment occur via losses during manufacturing (i.e. fugitive emissions) and through the use and disposal of products containing the chemical or use of the chemical itself. Because they are highly persistent, many PBTs are capable of long range transport and can be found in remote locations. There are many pathways through which PBTs may enter a waterbody, such as wastewater treatment plant effluent, stormwater, and atmospheric deposition.

4.0 Project Description

4.1 Project goals

The following goal will be added to the 2017/2018 project:

- Identify potential PBT chemicals in freshwater fish tissue to prioritize as target analytes in future PBT Monitoring projects.
- Provide information on a large suite of chemicals to support PBT List reprioritization and agency actions surrounding chemicals of concern.

4.2 Project objectives

The following objectives will be carried out to meet the additional project goals:

- A total of six upper-trophic level fish tissue samples collected from Lake Ozette, Lake Spokane, and Lake Washington will be sent to UWT CUW for non-targeted screening via QTOF LC-MS/MS of anthropogenic halogenated organic compounds.
- The resulting compound list from the non-targeted screening will be used to identify potential PBT chemicals to focus on in targeted analysis in future monitoring projects.

4.3 Information needed and sources

UWT CUW will use the mass spectral database Metlin for compound identification. Other open source mass spectral databases and libraries may be used if necessary. For compound

prioritization, estimated PBT lists from the literature will be used to identify potential priority chemicals. These lists (Brown and Wania, 2008; Howard and Muir, 2010; Strempel et al., 2012) are published in peer-reviewed journals.

4.4 Tasks required

The following tasks will be carried out for this project:

- Project manager will develop an interagency agreement (IAA) with UWT CUW for work described in this QAPP addendum.
- Project manager will submit fish tissue samples to UWT CUW in January 2018.
- UWT CUW will first conduct MS-only screen for widest range of compounds.
- Project manager will meet with UWT CUW after MS-only screen to discuss results and narrowing of compounds of interest.
- UWT CUW will conduct a MS/MS screen for a narrowed list of compounds.
- Project manager will again meet with UWT CUW to discuss MS/MS screen and determine whether any further compound identification is necessary (i.e., whether to invest in external reference standard for structure confirmation).
- UWT CUW will submit to project manager a short synopsis describing the method and results, as well as the resulting lists of compounds.
- Project manager will assess the results of the non-targeted screening and identify compounds of interest and priority for future targeted monitoring.
- Project manager will write draft report summarizing results and recommendations and route the draft report following Ecology's Environmental Assessment Program publication review procedures, and publish final report.

5.0 Organization and Schedule

5.1 Key individuals and their responsibilities

Table 1. Organization of project staff and responsibilities.

Staff (All EAP)	Title	Responsibilities
Debby Sargeant Toxics Studies Unit SCS Phone: 360-407-6775	Client and Supervisor for the Project Manager	Clarifies scope of the project. Provides internal review of the QAPP addendum and final report. Approves the final QAPP addendum. Manages personnel budget and staffing needs.
Jessica Archer SCS Phone: 360-407-6698	Client and SCS Manager	Reviews the project scope and budget, tracks progress. Provides internal review of the QAPP addendum and final report. Approves the final QAPP addendum.
Callie Mathieu Toxics Studies Unit SCS Phone: 360-4047-6965	Project Manager and Principal Investigator	Writes the QAPP addendum and final report. Coordinates with UWT CUW and reviews data. Analyzes and interprets data. Responsible for final report and project completion.
C. Andy James UWT CUW Phone: 253-254-7030 x8011	UWT CUW Sr. Research Scientist	Responsible for non-targeted screening by UWT CUW and reporting results to project manager.
Alan Rue Manchester Environmental Laboratory Phone: 360-871-8844	Acting Director	Reviews and approves the final QAPP addendum.
William R. Kammin Phone: 360-407-6964	Ecology Quality Assurance Officer	Reviews and approves the draft QAPP addendum and the final QAPP addendum.

EIM: Environmental Information Management database
QAPP: Quality Assurance Project Plan
SCS: Statewide Coordination Section
UWT CUW: University of Washington – Tacoma Center for Urban Waters

5.2 Special training and certifications

The UWT CUW laboratory staff have over three years of experience in performing non-targeted screening via Q-TOF LC-MS/MS. Staff operating the Q-TOF instrument have undergone 5 days of on-site training provided by Agilent. In addition, all UWT CUW laboratory staff are required to complete training courses on laboratory safety and managing laboratory chemicals. A full list of lab safety training requirements is included here: http://www.ehs.washington.edu/psotrain/.

5.4 Proposed project schedule

Table 2. Proposed Schedule for Completing Field and Laboratory Work and Completing Report.

Field and laboratory work	Due date	Lead staff
Field work completed	10/2017	Christopher Clinton
Samples sent to lab	01/2018	
Laboratory analyses completed	06/2018	
Final report		
Author lead / support staff	Callie Mathieu	
Schedule		
Draft due to supervisor	01/2019	
Draft due to client/peer reviewer	02/2019	
Final (all reviews done) due to publications coordinator	03/2019	
Final report due on web	04/2019	

5.5 Budget and funding

The laboratory budget for this project is $28,059. Table 3 presents the estimated costs for UWT CUW to complete the non-targeted screening. This project is funded by Ecology's PBT Monitoring Program budget.

Table 3. Estimated Costs of Non-Targeted Screening Analysis.

Item	Cost
Salaries	$15,425
Benefits	$5,530
Supplies	$908
Travel	$100
Indirect (26%)	$5,710
Other	$387
Analysis Total	**$28,059**

6.0 Quality Objectives

6.1 Data quality objectives

The data quality objective for this project is for completion of a non-targeted screening of anthropogenic halogenated compounds in 6 freshwater fish tissue samples via QTOF LC-

MS/MS. Data should be obtained that meets the Measurement Quality Objectives (MQOs) listed in Section 6.2.

6.2 Measurement quality objectives

Common MQOs have not been established for non-targeted screening via QTOF LC-MS/MS. However, UWT CUW laboratory has developed several internal QA/QC procedures and limits for this work. UWT CUW will follow the laboratory's Standard Operating Procedures for Non Targeted Analysis of Trace Organic Contaminants and ensure that the MQOs listed in Table 4 are met.

Table 4. Measurement Quality Objectives for Laboratory Analyses.

MQO	Precision	Bias	Sensitivity
Instrument Tune	< 2 ppm mass accuracy	--	Resolving power for tune solution ions: 118 m/z >5,900 322 m/z >60,000 622 m/z > 10,000 922 m/z > 12,000 1221 m/z > 12,500 1520 m/z >13,000 Tune solution ion response height 100k-400k (118 m/z > 40k)
Background ions	Retention time precision <0.1 min: triethyl citrate (RT 6.13 min), oleamide (RT 15.76 min), stearamide (RT 16.36 min), and an unidentified background ion (300.2019 Da @ 3.68 min)	--	--
Reference Mix	Retention time variation <0.1 min; Mass accuracy variation <5 ppm	--	Area response within ~20% of initial response
Replicates	--	Features present in ≥ 3 field replicates	--
Lab Blanks	--	Sample features present at abundance ≥ 5 times blank area abundance	---

The confidence achieved in compound identification can be classified according to a matrix developed by Schymanski et al. (2015) (Table 5). For this project, compounds will be identified in two phases: 1) MS-only scan and 2) MS/MS screen. The first MS-only scan will result in the widest range of compounds at a confidence level of 5 (lowest level of confidence). The next phase of the screening will employ an MS/MS fragmentation match to a mass spectral library. This second list will result in compounds identified to a confidence level of 2 (probable structure).

Table 5. Confidence Levels of Compound Identification.
Adapted from Schymanski et al. (2015).

Highest	1	Confirmed structure by reference standard
	2	Probable structure by library spectrum match
	3	Tentative candidate by structure, substituent, and class
	4	Unequivocal molecular formula
Lowest	5	Mass of interest

6.2.1 Targets for precision, bias, and sensitivity

6.2.1.1 Precision

Precision for the non-targeted screening method will be assessed by the MQOs listed in Table 4. For this type of data, precision is evaluated by examining instrument tuning, background signals, repeated injections of reference standards, and laboratory replicates.

Instrument tuning ensures consistent mass accuracy during a given analytical run and throughout the duration of the project. A check tune is performed prior to each analytical run, and the detector is re-tuned or re-calibrated if the mass error exceeds 2 ppm. The background signals listed in Table 4 are used to monitor chromatographic stability. A reference standard mix is analyzed every 8-12 samples to check chromatography and sensitivity during data acquisition. The mass accuracy limits and retention time limits are included in Table 4.

All fish tissue samples will be split by the laboratory for triplicate analyses. Only features (peaks of unique exact mass-retention time pairs) present in all three triplicate samples will be included for compound identification.

6.2.1.2 Bias

Laboratory bias for non-target data will be assessed through continuous injection of a reference solution during analytical runs. The reference solution contains 122 m/z and 922 m/z ions. If these two ions are not detected during an analytical run, the mass calibration cannot be ensured. Bias will also be assessed by the analysis of laboratory method blanks and instrument blanks. Laboratory blanks are prepared by the laboratory and processed in the same manner as the field

samples. Instrument blanks consist of solvents that are analyzed with the sample batch. Both types of blanks can provide information on contamination or bias in the laboratory. For this project, only features that are present at greater than or equal to five times the blank area abundances will be included in the analysis.

For non-target data, the identification and alignment of features is performed concurrently for all samples in a batch through Agilent MassHunter Profinder software (B.06.00). Features are defined as having mass height counts above the noise level (300) for positive or negative adducts. Alignment of features is based on matching retention time and mass within spans of 0.3 min and 30 ppm, respectively. Mass heights of ions must be above 5000 and appearing in all three triplicate samples. A recursive feature extraction will also be conducted on rescanned samples and extracted ions to capture features with heights greater than 3000 and match score greater than 50 that may have been missed during the first feature extraction.

6.2.1.3 Sensitivity

Sensitivity is a measure of the capability of a method to detect a substance. For non-detect data, sensitivity is assessed based on the detector resolving power, the results of repeated injections of reference standards, and by setting standards for minimum response of features. Measures to assess sensitivity and sensitivity limits are listed in Table 4.

The resolving power of the QTOF detector is typically 6,000 to 13,000 within the acquisition range. A standard tune solution is used to tune the instrument prior to each analytical run and specific targets for resolving power are set for individual masses in the tune solution (Table 4). The reference standard mix is run every 8-12 samples at a concentration of approximately 100 ug/L to check chromatography and sensitivity during data acquisition. Area counts are monitored and expected to be within 20% of initial sensitivity. Features with a mass height above 5,000 (S/N ~17) in the sample are included for further compound identification.

6.2.2 Targets for comparability, representativeness, and completeness

6.2.2.1 Comparability

To facilitate comparability of the data generated by this project and potential related future projects, field sampling will follow standardized operating procedures listed in Section 8.2. The following UWT CUW SOPs will be followed:

- SOP for Accelerated Solvent Extraction
- SOP for Quadrupole Time of Flight Liquid Chromatography Dual Mass Spectrometry (QTOF-LC-MS/MS) Setup, Operation, and Data Analysis: Non Targeted Analysis of Trace Organic Contaminants

6.2.2.2 Representativeness

Fish samples will be analyzed as 3-5 fish composites in order to integrate variability within a waterbody and among individual fish, providing a representative sample of that species/size and waterbody.

Study locations for this project likely to be impacted by urban or WWTP effluent inputs were targeted to identify occurrence of anthropogenic halogenated organic compounds. One waterbody was selected as a reference site, to represent concentrations occurring from atmospheric deposition. Lakes and reservoirs were selected as target waterbodies to obtain samples integrating many sources within a waterbody (e.g., tributaries and storm water.).

6.2.2.3 Completeness

The project manager will consider the study to have achieved completeness if 95% of the samples are analyzed acceptably.

7.0 Study Design

Ecology collected freshwater fish tissue from two urban waterbodies and one reference waterbody in October 2017 for targeted analysis of halogenated and organophosphate flame retardants, as documented in the original QAPP. This QAPP addendum describes additional testing of a subset of the fish tissue samples. Six homogenized fillet tissue samples of upper trophic level freshwater fish will be sent to UWT CUW for non-targeted screening of anthropogenic halogenated organic compounds by QTOF LC-MS/MS.

The non-targeted screening will follow the workflow presented in Figure 1 to result in a list of compounds present in the fish tissue that may potentially exhibit PBT characteristics. The halogenated compounds identified will then be prioritized by the relative intensity and prevalence of the compounds in the samples analyzed, and compounds that are on estimated PBT lists of commercial chemicals (Howard and Muir, 2010; Strempel et al., 2012; Brown and Wania, 2008). This prioritized list of compounds present in the fish tissue will then be used for recommendations for future targeted monitoring studies.

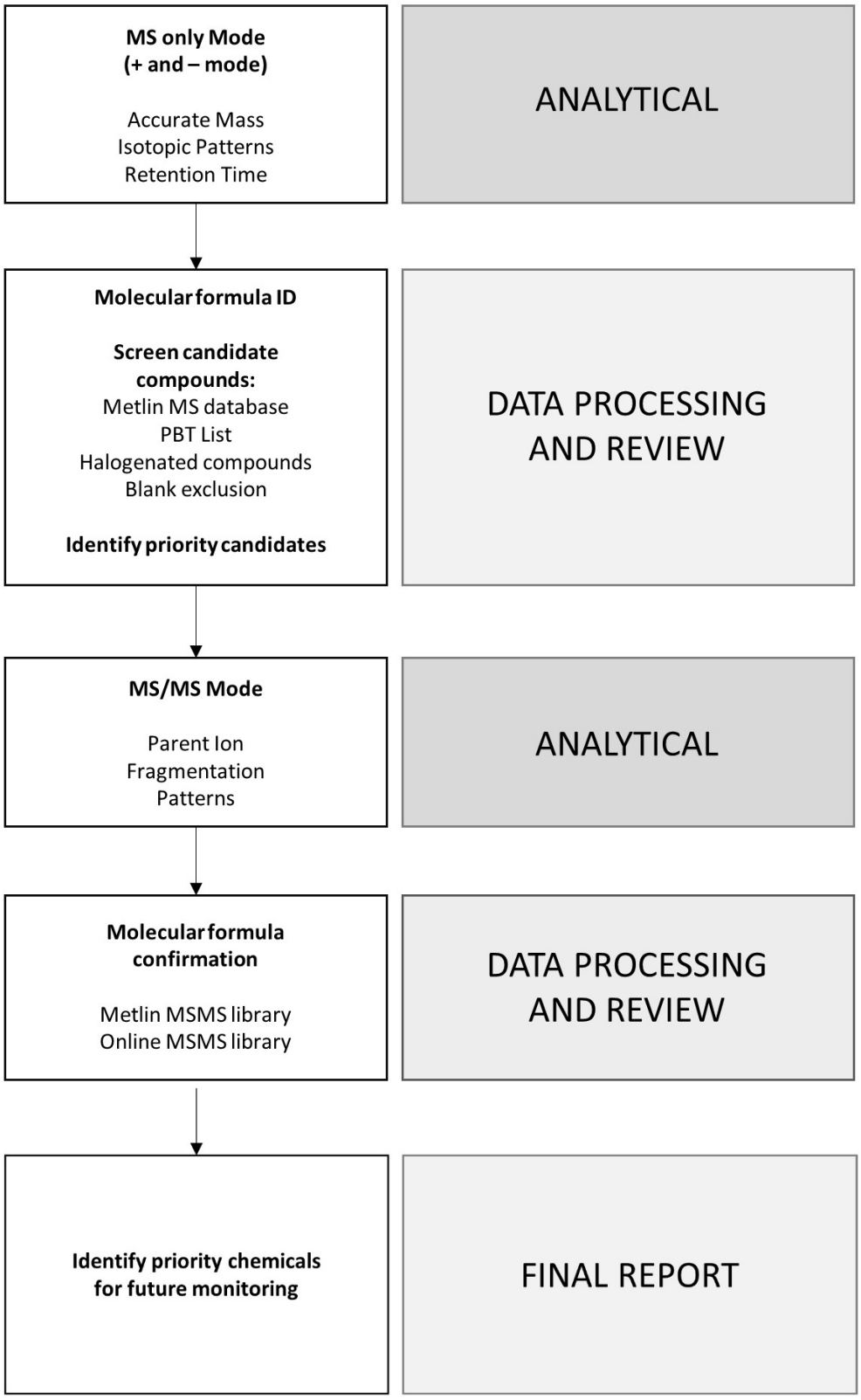

Figure 1. Simplified Work Flow for Non-Targeted Screening of Freshwater Fish Tissue Samples.

7.2.1 Sampling locations and frequency

Archived fish fillet samples collected from Lake Ozette, Lake Spokane, and Lake Washington will be analyzed for this non-targeted screening. Fish samples were collected in October 2017 under the original QAPP. Two composites of an upper trophic species per site will be submitted for analysis.

7.2.2 Field parameters and laboratory analytes to be measured

This project will identify anthropogenic halogenated organic compounds in freshwater fish tissue samples. Non-detect data will consist of a list of compounds and relative abundance of each compound. Concentrations of compounds in samples will not be measured or reported.

7.4 Assumptions in relation to objectives and study area

This project makes the assumption that the QTOF LC-MS/MS non-targeted screening method will be successful in identifying anthropogenic halogenated organic compounds in homogenized fish fillet tissues.

8.0 Field Procedures

8.3 Containers, preservation methods, holding times

Table 6 describes the sample matrix, minimum quantity required, container size, preservation, and holding time for the samples.

Table 6. Sample Container, Preservation Methods, and Holding Times.

Analysis	Matrix	Minimum Quantity Required	Container	Preservative	Holding Time
non-targeted screening	fish tissue	50 g ww	8 oz glass jar	freeze at ≤ -10° C	1 year frozen

9.0 Laboratory Procedures

9.2 Sample preparation method(s)

Fish tissue samples will be homogenized by Ecology following procedures outlined in the original QAPP. UWT CUW will utilize an accelerated solvent extraction process on the samples prior to analysis following the laboratory's SOP for Accelerated Solvent Extraction.

9.3 Special method requirements

The non-target screening will be performed on an Agilent QTOF LC-MS/MS following UWT CUW Standard Operating Procedures listed in Section 6.2.2.

9.4 Laboratories accredited for methods

Currently, no laboratories are accredited for non-targeted screening. An Ecology waiver for accreditation will be obtained for this project.

10.0 Quality Control Procedures

UWT CUW will be expected to perform the quality control procedures listed in Table 7 and described in Section 6. The reference standard mix included in each analytical run as a check on mass accuracy, compound identification, and response will be required to include at least one halogenated organic compound. Sample extracts will be spiked with a known mass of labelled standard as a check on instrument response and matrix interference. Method blanks and instrument blanks will be run as listed in Table 7. Each sample will be split into triplicates by the laboratory and analyzed separately.

10.1 Table of laboratory quality control

Table 7 provides the laboratory QC procedures required for this project. Field QC procedures are described in the original QAPP.

Table 7. Quality Control Samples and Frequency.

Analysis	Matrix	Laboratory					
		Check tune	Method blank	Instrument blank	Lab split (triplicate)	Check standard	Reference standard mix
non-targeted screening	fish tissue	each analytical run	1 per batch	every 8-12 samples	each sample	every 8-12 samples	each sample

Batch = 20 samples or fewer.
[1] Calibrant mix

10.2 Corrective action processes

The project manager will meet with UWT CUW staff to discuss the results of the first phase of screening (MS-only). At that meeting any issues with the method or analysis will be discussed as well as focus parameters for further prioritization during the second phase (MS/MS screen). A second meeting will occur between UWT CUW and the project manager to review the MS/MS screen and determine whether any additional compound identification is necessary.

11.0 Management Procedures

11.1 Data recording and reporting requirements

Data generated from the Q-TOF LC-MS/MS non-targeted screening will not be uploaded into EIM due to the non-quantitative nature of the data. The final deliverable from UWT CUW will be stored on the Environmental Assessment Program's Toxics Technical Coordination Team Sharepoint site. This site currently houses passive sampler data that does not get stored in the EIM database. The project manager will make the data available to the public upon request. Results from the non-targeted screening will be included in the final report for this project.

11.2 Laboratory data package requirements

UWT CUW will provide a written synopsis of the results of the non-targeted screening. The synopsis will include (1) an evaluation of the success of the method, (2) a list of chemicals identified through the screening, and (3) recommendations for future steps in the effort to identify chemicals for further evaluation and monitoring.

UWT CUW will provide the list of chemicals in an Excel list format. Compounds will be reported with the following data: compound name, formula, theoretical mass, CAS # (if available), RT (min), log K_{ow}, identification confidence level (based on Schymanski et al. (2015)), relative abundance, and mass error (ppm).

The data package from UWT CUW will include documentation of QA/QC tests for each batch, including check tune results for each run. Instrument print outs of check tune results will be in pdf format.

11.3 Electronic transfer requirements

UWT CUW will transfer all deliverables via email to the project manager.

12.0 Audits and Reports

The results of the non-targeted screening will be included as a separate section in the final report for the original study. The final report will include a discussion of the non-targeted screening method, resulting lists of chemicals from the screening, and recommendations on how to use this information to inform future monitoring.

13.0 Data Verification

13.2 Laboratory data verification

The project manager will review the results of the non-targeted screening and determine whether MQOs were met and SOPs were followed. The project manager will be responsible for the final acceptance of the results. The resulting lists of compounds identified by the non-targeted screening, as well as the written synopsis provided by UWT CUW, will be assessed for completeness and reasonableness.

14.0 Data Quality (Usability) Assessment

14.1 Process for determining project objectives were met

After the screening results and synopsis have been reviewed, the project manager will determine if the results are of sufficient quality to make determinations and decisions for which the study was conducted. The data from the laboratory's QC procedures will provide information to determine if MQOs have been met. The project final report will discuss data quality and whether the project objectives were met. If limitations in the data are identified, they will be noted.

14.5 Documentation of assessment

Documentation of assessment will occur in the final report.

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