# Monitoring Strategies for Constituents of Emerging Concern (CECs) in California's Aquatic Ecosystems

## Recommendations of a Science Advisory Panel

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# PREFACE

In October 2020, the Science Advisory Panel for Chemicals of Emerging Concern (CECs) in California's Aquatic Ecosystems ("CEC Ecosystems Panel") was reconvened at the request of the State Water Resources Control Board (State Water Board) to provide unbiased science-based recommendations for monitoring strategies of chemicals of emerging concern in oceanic, brackish, and fresh waters across the State that receive discharge of treated municipal wastewater effluent and stormwater. The CEC Ecosystem Panel was comprised of 7 members of which six members also served on the previous CEC Ecosystems Panel, whose final recommendations were published in April 2012. Funding for the CEC Ecosystems Panel effort was provided by the SWRCB and the Ocean Protection Council (OPC).

The Southern California Coastal Water Research Project (SCCWRP) was selected to convene the Panel, facilitate and manage their activities and to coordinate the writing and submission of this report. Dr. Charles Wong served as the Project Manager and Lead Facilitator for SCCWRP. Ms. Erica Kalve served as Contract Manager for the SWRCB, while Ms. Holly Wyer (2020-2021) and Ms. Kaitlyn Kalua (2021-present) served as Contract Managers for the OPC. A Steering Committee of 13 advisors representing the discharger, NGO, regulator, and resource communities was established to provide stakeholder input to the process. A series of virtual and two physical meetings were held over a 2-year period (the final virtual meeting scheduled for December 12, 2022) for the Panel to formulate their recommendations. This report, targeted to the stakeholder audience described above, represents the culmination of the CEC Ecosystems Panel's work.

# ACKNOWLEDGMENTS

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Members of the Panel and SCCWRP would like to acknowledge members of the Interagency Advisory Committee formed to serve as a state-wide liaison for their respective agencies. These advisors are:

- Jeremiah Puget (North Coast Regional Water Board)
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# EXECUTIVE SUMMARY

Constituents of emerging concern (CECs) encompass a vast number of chemical substances that are generally unregulated in the U.S. or have limited regulation in environmental media (e.g., air, water, sediment, and biota) around the world. CECs may include a wide variety of substances ranging from pharmaceuticals to flame retardants or per- and polyfluoroalkyl substances (PFAS) to newly registered contemporary use pesticides to newly developed commercial products such as nanomaterials. Advances in qualitative and quantitative analytical chemistry have allowed detection in various environmental media and have led to initiatives to estimate the potential hazard of CECs. A multitude of chemical substance that may be qualitatively identified cannot be quantified due to lack of standards or robust methods of measurement. Thus, regulators in the State of California have been trying to narrow the focus of chemical substance screening in the aquatic environment to compounds that have the greatest potential to pose a risk to human and ecological health.

To assist in this process, a previous Science Advisory Panel developed and recommended a risk-based screening framework to identify CECs for monitoring in California's aquatic ecosystems in 2012. The 2012 Panel applied the framework using existing information to three representative receiving water scenarios to identify a list of appropriate CECs for initial monitoring, developed an adaptive phased monitoring approach and suggested development of bioanalytical screening and predictive modeling tools to improve assessment of the presence of CECs and their potential risk to the environment.

In order to consider knowledge gained during the last decade from ongoing CEC monitoring within the State of California but also from research outside the state, the California Water Resources Control Board (State Water Board) in conjunction with the Ocean Protection Council and a group of stakeholder advisors re-convened a group of leading scientists in October 2020 to address the issues associated with CECs in the State's aquatic systems. The 2022 Panel was comprised of seven experts in chemistry, biochemistry, toxicology, chemical and risk assessment, engineering, and coastal and marine environmental health science. The 2022 Panel was provided with six specific charge questions, but was generally tasked to review the occurrence, relevance, and quantification of CECs with a main focus on ambient surface fresh, marine, and estuarine water ecosystems with the goal to provide recommendations for development of a monitoring program of CECs in fresh, estuarine, and oceanic water bodies of California.

As one source of CEC occurrence data, the 2022 Panel considered the dataset of organic chemicals assembled by the Aquatic Science Center (ASC) for the State Water

Board augmented (Sutton et al. 2022). This dataset covered a period from 2005 to 2022 and also included information on chemicals in sediment and biota. The CEC dataset covered over 420 chemicals in 11 classes with measured values in fresh, estuarine, and marine waters, which were evaluated individually by the Panel. Broad classes defined by similar chemical structures (e.g., bisphenols), and/or function or purpose in society (e.g., pharmaceuticals) were considered. Building upon this dataset, the Panel established a quality assurance workflow for CEC monitoring data and a risk-based screening framework. The Panel also used additional multimedia-occurrence data considering other state, national and international sources reporting on CECs not currently included in California's ongoing previous or existing monitoring programs. In addition, the Panel considered additional sources on toxicity to sensitive species and assembled toxicity threshold values for these CECs. Applying this framework will result in a preliminary monitoring prioritization, a refined monitoring prioritization, and a final recommended monitoring list or programs.

The Panel held multiple virtual meetings and two in-person meetings to formulate their approach and recommendations. This report provides the results from the Panel's deliberations, including four products intended to assist the State in developing a monitoring process for CECs based on sound, up-to-date scientific principles.

**Product #1: Guidance to structure, quality assurance and visualization of CECs covered by the existing State Water Board CEC dataset**

Building upon recommendations of the 2012 Panel Report, the State Water Board compiled CEC monitoring data in a CEC dataset that considered CEC monitoring data from various State Water Board initiatives as well as sister agencies within California Environmental Protection Agency, California Natural Resources Agency including compliance monitoring. The State Water Board dataset used in this report was assembled in a data synthesis report prepared by ASC (Sutton et al. 2022) and was based on monitoring records for 11 classes of CECs analyzed from 2005 to 2022 in California's ambient aquatic ecosystems. The majority of the records were for surface waters (61%); sediment, and influents/effluents constitute 30%. The Panel focused its assessment on the surface water records in fresh, estuarine, and marine settings. Pesticides and pharmaceuticals constituted the majority of the chemicals analyzed for in freshwater and estuarine samples (67 and 61%, respectively). A large number of records were available for surface waters (280,653 in freshwater) and geographic coverage was very good with results from up to 3,622 sampling stations. However, only 12% (freshwater) to 30% (marine waters) of the records reported detectable concentrations. But the detections do not necessarily imply risk or hazard, nor do non-detects necessarily imply lack of risk or hazard.

The Panel reviewed the status and quality of the dataset provided and established a quality assurance workflow for CEC monitoring data. To assess sources, pathways, and rate of inputs leading to the presence of classes of CECs in the fresh, estuarine, and marine water ecosystems, the Panel utilized and expanded the CEC dataset provided by the State Water Board. Considering the wide range of physico-chemical properties of these CECs, the Panel considered different matrices (i.e., dissolved and total concentrations in ambient fresh, wastewater, estuarine and marine water, tissues and sediments) to assess the relevance of specific CECs for the aquatic environment. In addition, a class-based approach was used to summarize and visualize the data also allowing a quick assessment of temporal and geographical variations of individual CECs or classes of CECs.

There was a substantial amount of CEC data collected since the Panel was last convened. However, since the data came from many different sources with various data quality standards, this not only took a substantial amount of time to try to reconcile the differences, but also highlighted the need for statewide guidance on data quality objectives for CEC monitoring. For example, the lack of the latitude/longitude information for 27% of surface water results severely limited the utility of the data. Further complicating the records, detection limits for individual analytes often spanned several orders of magnitude, were listed as zero, or left blank. This seems to have been due to multiple agencies providing data with different reporting limits. When calculating the MEC (i.e., the 90th percentile) for a CEC, the Panel utilized the available detection limit information and substituted the median CEC-specific detection limit for non-detect samples of that CEC, as long as that CEC was detected in at least one sample. This resulted in 90th percentiles for the substituted datasets being higher than the 90th percentiles based only on reported data for many pesticides and pharmaceuticals. On the other hand, it enabled better use of the available data for highly censored chemicals that had at least some detectable levels. Visualization of the data enables more detailed evaluation of the including geographic coverage for detects and non-detects, frequency of sampling, and temporal trends in concentrations.

A total of 423 CECs were reported across all media. These CECs were categorized into eleven classes: Pesticides, pharmaceuticals, alkyl phenols/alkyl phenol ethoxylates (AP/APEs), phthalates, polybrominated diphenyl ethers (PBDEs), brominated flame retardants (BFRs), PFAS, personal care products (PCPs), bisphenols, organophosphate esters (OPEs), and natural toxins (microcystins and marine toxins) (Appendix C. Table C.1). Pharmaceuticals constituted the largest group of individual CECs in freshwater (108) and estuarine waters (83), although only five were reported in marine waters. Pesticides were the next largest group ranging from 44 compounds in marine water to 108 in freshwater. PBDEs were the third largest group in water due to reporting for 51 congeners. Highest detection frequencies (DFs) for PBDE in freshwaters were for congeners 15, 28, 47, 49, 99, 100, 119, 140 and 153.

The Panel suggests that the State Water Board categorize the quality of data and potential uses of the data from each of the databases such that the expected shortcomings of the data quality and acceptance criteria are documented as part of applying the proposed prioritization framework. That will enable the State Water Board and stakeholders to determine the utility of data from the various sources and databases.

**Product #2: Guidance to use other sources to inform a CEC monitoring program**

The Panel also used additional multimedia-occurrence data considering other state, national and international sources reporting on CECs not currently included in California's ongoing previous or existing monitoring programs. To inform what CECs should be considered in monitoring programs in California, occurrence data sources beyond the State Water Board dataset, both within the state of California and outside of it, can be used to identify applicable analytical methods and reporting limits for these CECs. In addition to the use of target analyses methods, important known and unknown biological effects for specific or classes of CECs could be assessed using non-targeted analyses (NTA). Non-targeted analyses are highly valuable when developing comprehensive programs for identifying potential substances of environmental risk. Non-targeted analyses generally include mass spectrometric techniques, bioassays, and iterative combinations of instrumental and bioanalytical techniques. These approaches need to be critically evaluated to determine how well they assess biological effects of classes of CECs to sentinel species in fresh, estuarine, and marine water ecosystems.

In total 133 compounds were included in the "new CECs" list. A subset of these were assessed by the Panel. Sixteen compounds were selected for prioritization including 6PPD-quinone, a compound highly toxic to coho salmon (Oncorhynchus kisutch) and salmonid species.

**Product #3: An updated risk-based approach to assess and identify CECs for monitoring in California receiving waters**

Given the substantial time associated with the cleanup of the CEC dataset, the Panel refocused on demonstrating a "proof of concept" for an updated and expanded risk- and occurrence-based monitoring prioritization framework, providing the Water Boards with a model, and a road map to use when developing the monitoring prioritization and broader implementation, including dataset updates, as part of the statewide CEC Program.

The Panel expanded the previously developed risk-based screening framework, which includes four primary steps:

1. Toxicity assessment: developing monitoring trigger levels (MTLs) for CECs that pose the greatest potential risk to aquatic systems based on published effects concentrations.
2. Preliminary monitoring prioritization: rating short-lists of CECs based on measured environmental concentrations (MECs) and trends for CECs for which MTLs could be estimated.
3. Refined monitoring prioritization: Identify those CECs that are relevant based on sample size, the identified trends (geographical and temporal), monitoring trigger quotient (MTQ) having the greatest potential to pose a risk by comparing MECs to MTLs. CECs with a monitoring trigger quotient (MTQ = MEC/MTL) greater than "1" were identified for monitoring.
4. Recommended Monitoring Program: specify the nature of local, regional and state-wide monitoring efforts.

To conduct the preliminary monitoring prioritization, available data and MTLs are used to calculate an $MTQ_{detect}$, $MTQ_{sub}$, and trend. If data are available, MTQs and trend can be calculated for all environmental media (e.g., fresh, marine water, estuarine water, sediment, and tissue). The preliminary monitoring prioritization process categorizes CECs as either needing to be retained for possible inclusion in a monitoring program or eliminated from consideration in a current monitoring program. CECs that are eliminated from consideration in a monitoring program based on current data can be evaluated again using the preliminary monitoring prioritization screening process if additional data are collected or if MTLs change. CECs that are retained for possible inclusion in a monitoring program are categorized as having either 'High', 'Moderate' or 'Low' monitoring priority.

The refined monitoring prioritization framework consists of criteria specified in an MTQ selection Table (Table 6.2.1) and 10 decision tree diagrams (Appendix G, Figures G.1 through G.10). The MTQ selection table is used to determine whether the $MTQ_{detect}$ or $MTQ_{sub}$ will be used in the monitoring refinement prioritization. Each of the decision diagrams corresponds to one of the 10 preliminary monitoring prioritization outcomes shown in Figure 5.3. The MTQ selection table was necessary to address the uncertainty regarding MDLs in the current State Water Board dataset.

Application of the refined monitoring prioritization framework consists of first applying a MTQ selection table to determine which MTQ will be used in the refinement. Once either $MTQ_{detect}$ or $MTQ_{sub}$ is selected, the decision tree diagram corresponding to a

CEC's preliminary monitoring prioritization category is used to refine the prioritization. In addition, refinement may be required for the MTL as discussed above where more accurate thresholds may be identified from the literature or from other studies in the database that have appropriate QA/QC (i.e., measured chemistry of exposure). Application of the refinement process was executed for five example freshwater CECs and three example marine CECs, all with a 'High' preliminary monitoring prioritization category.

The two-stage risk-based screening framework is not uniquely applicable to the State Water Board CEC dataset. If other datasets have available monitoring data, the screening and prioritization process can be applied to those as well.

**Product #4: Establishing a sound foundation for a state-wide and regional CEC monitoring program in California**

- Given the substantial time associated with the cleanup of the CEC dataset, the Panel refocused on demonstrating a "proof of concept" for an updated and expanded risk- and occurrence-based monitoring prioritization framework, providing the Water Boards with a model, and a road map to use when developing the monitoring prioritization and broader implementation, including dataset updates, as part of the statewide CEC Program.
- The overall recommendation for the State Water Board CEC Program is to complement the continuing risk-based monitoring approach with temporal and spatial evaluations, improve the quality of data reported to the State Water Board, regularly update the monitoring trigger levels (MTLs) as new CEC monitoring and toxicology information become available, develop a pilot biomonitoring program focused on early identification of effects in ambient waters, work with a future Ambient Ecosystems CEC Advisory Panel or an equivalent process for expert review, and ultimately update existing policy and monitoring requirements to update the State's approach to CEC monitoring and management, and to guide a state-wide CEC monitoring program for receiving waters.
- An overarching concern that has crystalized over the past two years for the Panel is the tremendous challenge of using the existing disparate systems to collect and compile occurrence data in statewide database. After consulting with state agencies, it may not be possible to create a system that assures that all of the CEC occurrence data entered into such a statewide system can be of uniform high quality. If that cannot be accomplished, then the Panel sees limited utility to such a compilation for the purpose of monitoring CECs. As pointed out in the report (see Chapters 3, 7 and 8), the Panel believes a

more focused statewide monitoring program dedicated to evaluating CECs that relies on more than occurrence data will be a more efficient use of resources and provide the State an abundance of information about CECs in, and their possible effects on, California's aquatic ecosystems.

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# ACRONYMS

List of acronyms used in this report.

| Acronym | Term |
|---|---|
| **AhR** | Aryl Hydrocarbon Receptor |
| **AOP** | Advanced Oxidation Process |
| **AP/APEs** | Alkyl Phenols/Alkyl Phenol Ethoxylates |
| **ASC** | Aquatic Science Center |
| **CECs** | Constituents of Emerging Concern |
| **CEDEN** | California Environmental Data Exchange Network |
| **DCA** | 3,4-Dichloroaniine |
| **DDT** | Dichlorodiphenyltrichloroethane |
| **DEET** | *N*,*N*-Diethyl-*meta*-Toluamide |
| **DF** | Detection Frequency |
| **DPG** | 1,3-Diphenyl Guanidine |
| **DWR** | Department of Water Resources |
| **E2** | 17β-estradiol |
| **EDA** | Effects-Directed Analysis |
| **EDCs** | Endocrine Disrupting Compounds |
| **EE2** | 17α-ethinyl estradiol |
| **EPA WQX** | United States Environmental Protection Agency, Water Quality Exchange |
| **ER** | Estrogen Receptor |
| **GC-MS** | Gas Chromatography-Mass Spectrometry |
| **GR** | Glucocorticoid Receptor |
| **GWRC** | Global Water Research Coalition |
| **hER** | Human Estrogen Receptor |
| **LC50/EC50** | Lethal Concentration/Effect affecting 50% |
| **LC-MS** | Liquid Chromatography-Mass Spectrometry |
| **LC-QTOF** | Liquid Chromatography-Quadrupole Time-of-Flight Mass Spectrometer |

| | |
|---|---|
| **LOEC** | Lowest Observable Effect Level |
| **MEC** | Measured Environmental Concentration |
| **MDL** | Method Detection Limit |
| **MIE** | Molecular Initiating Event |
| **MS** | Mass Spectrometry |
| **MTL** | Monitoring Trigger Level |
| **MTQ** | Monitoring Trigger Quotient |
| **ND** | Non-Detect |
| **NIEHS/NTP** | National Institute of Environmental Health Sciences/National Toxicology Program |
| **NGO** | Non-Governmental Organization |
| **NOEC** | No Observable Effect Concentration |
| **NTA** | Non-Targeted Analysis |
| **NWQMC** | National Water Quality Monitoring Council |
| **OPC** | California Ocean Protection Council |
| **OPEs** | Organophosphate Easters |
| **PAHs** | Polycyclic Aromatic Hydrocarbons |
| **PBDEs** | Polybrominated Diphenyl Ethers |
| **PCBs** | Polychlorinated Biphenyls |
| **PCPs** | Personal Care Products |
| **PEC** | Predicted Environmental Concentration |
| **PFAS** | Per- and Polyfluoroalkyl Substances |
| **PFOA** | Perfluorooctanoic Acid |
| **PFOS** | Perfluorooctanoic Sulfonic Acid |
| **PNEC** | Predicted No Effect Concentration |
| **6PPD-quinone** | *N*-(1,3-Dimethylbutyl)-*N'*-phenyl-*p*-phenylenediamine-quinone |
| **qPCR** | Quantitative Polymerase Chain Reaction |
| **QA** | Quality Assurance |
| **QA/QC** | Quality Assurance/Quality Control |
| **RNA** | Ribonucleic Acid |

| | |
|---|---|
| **SDWIS** | Safe Drinking Water Information System |
| **State Water Board** | California State Water Resources Control Board |
| **TCDD** | 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin |
| **USEPA** | United States Environmental Protection Agency |
| **USGS NWIS** | United States Geological Survey, National Water Information System |
| **WHO** | World Health Organization |
| **WWTP** | Wastewater Treatment Plant |

# DEFINITIONS

List of key terms used in this report.

| Definition | Term |
|---|---|
| **2022 Panel (or "Panel" without a year)** | Current Ambient Ecosystems CEC Advisory Panel II authoring this report, with membership as listed in Chapter 1.2, also named "the Panel". Previous advisory panels are listed by year e.g., "2012 Panel" refers to the Science Advisory Panel of Anderson et al. (2012), Monitoring Strategies for Chemicals of Emerging Concern (CECs) in California's Aquatic Ecosystems: Recommendations of a Science Advisory Panel, SCCWRP Technical Report 692 |
| **ASC Report** | CEC data synthesis considering monitoring data collected as part of the CEC Initiative published as Sutton et al. (2022) |
| **State Water Board Dataset** | The ASC Report's Data Synthesis, as described in the ASC Report and introduced in Chapter 2 |
| **CEC Dashboard** | The State Water Board Dataset that had undergone revision by the State Water Board as described in Chapter 2.1.1 and Appendix B |
| **Preliminary Monitoring Prioritization** | The CEC Dashboard that has been assessed by the screening algorithm described in Chapter 5.2 and results presented in Chapter 6.1 |
| **Refined Monitoring Prioritization** | Prioritization of CECs from the Preliminary Monitoring Prioritization list that have been assessed by the screening algorithm described in Chapter 6.2 |
| **MEC** | The $90^{th}$ percentile of the Measured Environmental Concentration from datasets, or subsets thereof (e.g., $MEC_{detect}$) as noted, unless explicitly stated otherwise in this report (e.g., "Mean MEC") |

| | |
|---|---|
| **$MEC_{detect}$** | The 90th percentile of only the detected concentrations of a CEC (all non-detect samples excluded) for the entire time period studied (2005-01-01 to 2021-12-31) |
| **$MEC_{sub}$** | The 90th percentile of all samples of a CEC, including both concentrations of detected and non-detect samples, and substituting the median MDL for non-detect samples of that CEC for the entire time period studied (2005-01-01 to 2021-12-31) |
| **$MEC_{detect,2010}$** | The 90th percentile of only detected concentrations of a CEC measured between 2005-01-01 and 2010-12-31 |
| **$MEC_{detect,2015}$** | The 90th percentile of only detected concentrations of a CEC measured between 2011-01-01 and 2015-12-31 |
| **$MEC_{detect,2021}$** | The 90th percentile of only detected concentrations of a CEC measured between 2016-01-01 and 2021-12-31 |
| **$MEC_{sub,2010}$** | The 90th percentile of all samples of a CEC including concentrations of detected samples and non-detect samples, and substituting the median MDL for that CEC measured between 2005-01-01 and 2010-12-31 for non-detect samples |
| **$MEC_{sub,2015}$** | The 90th percentile of all samples of a CEC including concentrations of detected samples and non-detect samples, and substituting the median MDL for that CEC measured between 2011-01-01 and 2015-12-31 for non-detect samples |
| **$MEC_{sub,2021}$** | The 90th percentile of all samples of a CEC including concentrations of detected samples and non-detect samples, and substituting the median MDL for that CEC measured between 2016-01-01 and 2021-12-31 for non-detect samples |
| **$MEC_{sub}$** | The 90th percentile of all samples of a CEC including concentrations of detected samples and non-detect samples, and substituting the median MDL for that CEC measured between 2005-01-01 and 2021-12-31 for non-detect samples |

| | |
|---|---|
| **$MTQ_{detect}$** | The monitoring trigger quotient based on the MEC (90th percentile) of only detected concentrations of a CEC |
| **$MTQ_{sub}$** | The monitoring trigger quotient based on the MEC (90th percentile) of all samples of a CEC including concentrations of detected samples and non-detect samples, and substituting the median MDL for non-detect samples of that CEC for the entire time period studied (2005-01-01 to 2021-12-31) |
| **$MTQ_{detect,2010}$** | The monitoring trigger quotient based on the $MEC_{detect,2010}$ |
| **$MTQ_{detect,2015}$** | The monitoring trigger quotient based on the $MEC_{detect,2015}$ |
| **$MTQ_{detect,2021}$** | The monitoring trigger quotient based on the $MEC_{detect,2021}$ |
| **$MTQ_{sub,2010}$** | The monitoring trigger quotient based on the $MEC_{sub,2010}$ |
| **$MTQ_{sub,2015}$** | The monitoring trigger quotient based on the $MEC_{sub,2015}$ |
| **$MTQ_{sub,2021}$** | The monitoring trigger quotient based on the $MEC_{sub,2021}$ |

# 1. INTRODUCTION

Modern life relies on availability and utilization of natural and synthetic chemical substances which may enter ground and surface waters through runoff, industrial and municipal waste discharges, atmospheric deposition, or through releases from septic systems (Figure 1.1). While new chemical substances are constantly introduced and others phased out, the concept of humans altering their exposure to these materials through manipulation of the natural system is as long and rich as human history. Today, nearly any imaginable chemical substance can be detected in water given ample sample volume and availability of purified standard material for instrument calibration.

Constituents of emerging concern (CECs) encompass a vast number of chemical substances that are generally unregulated in the U.S. or have limited regulation in environmental media (e.g., air, water, sediment, and biota) around the world. CECs may include a wide variety of substances ranging from pharmaceuticals to flame retardants or per- and polyfluoroalkyl substances (PFAS) to newly registered contemporary use pesticides to newly developed commercial products such as nanomaterials. Generally, with the notable exception of new industrial or pharmaceutical compounds, many of these chemical substances have likely been present in water bodies, sediments, and tissues for many years and even decades but at concentrations that were not detectable by commonly used analytical methods. However, advances in qualitative and quantitative analytical chemistry have allowed detection in various environmental media and have led to initiatives to estimate the potential hazard of CECs. A multitude of chemical substances that may be qualitatively identified cannot be quantified due to lack of standards or robust methods of measurement. Thus, regulators in the State of California have been trying to narrow the focus of chemical substance screening in the aquatic environment to compounds that have the greatest potential to pose a risk to human and ecological health.

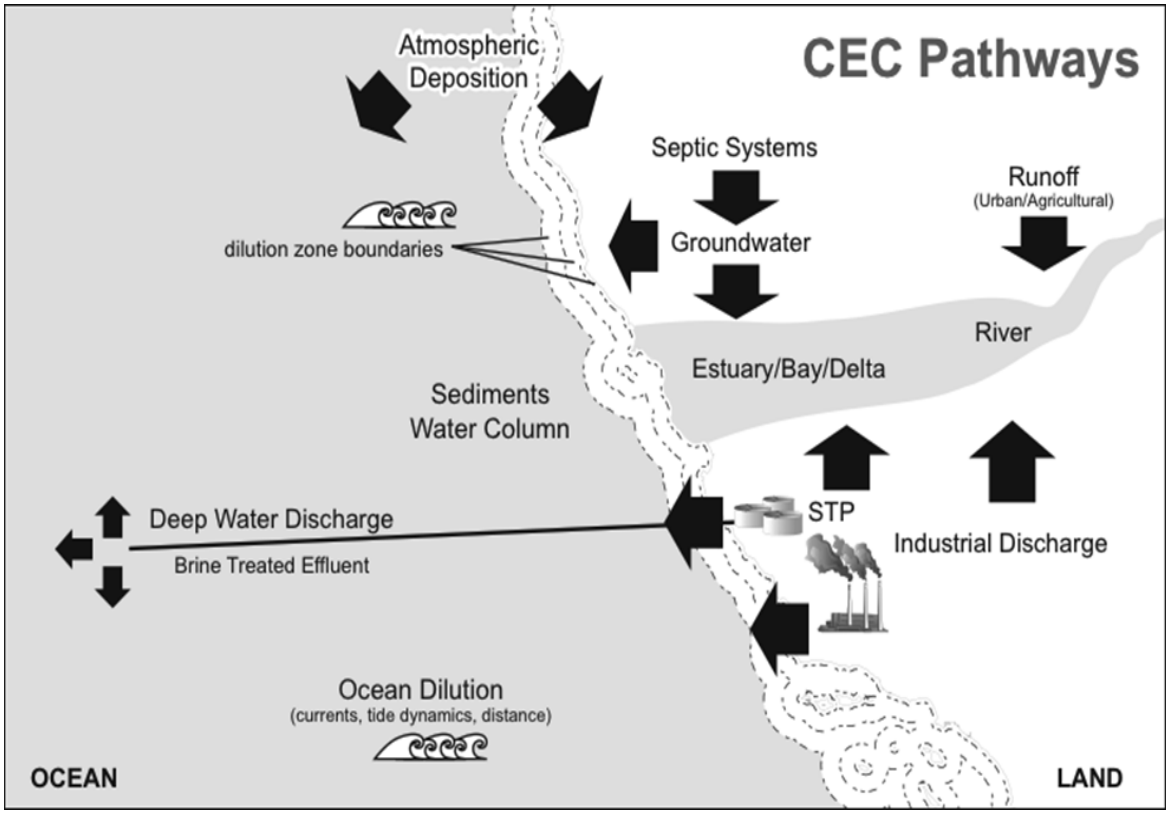


**Figure 1.1. Conceptual model of potential sources and pathways for the introduction of constituents of emerging concern (CECs) into the aquatic environment.**

## 1.1 The Statewide CEC Program

In October 2009, the State of California Water Resources Control Board (State Water Board) provided support for a scientific advisory panel to review existing scientific literature on CECs in aquatic ecosystems; determine the state of the current scientific knowledge regarding the risks that CECs in freshwater and marine water pose to human health and aquatic ecosystems; and provide recommendations on improving the understanding of CECs for the protection of public health and the environment. Seven experts were vetted and convened as the CEC Ecosystems Panel (2012 Panel) to provide information and recommendations on CECs in coastal and marine ecosystems, which was subsequently tasked to expand the scope to include freshwater ecosystems. The 2012 Panel collaborated with stakeholders, who provided their perspective of the water quality issues and additional information during the development of their recommendations. In their final report entitled 'Monitoring Strategies for Chemicals of Emerging Concern (CECs) in California's Aquatic Ecosystems: Recommendations of a Science Advisory Panel' (SCCWRP Technical Report 692, Anderson et al. 2012), the 2012 Panel recommended a risk-based screening framework to identify CECs for monitoring. The 2012 Panel applied the framework using existing information to three representative receiving water scenarios to identify a list of appropriate CECs for initial monitoring, developed an adaptive phased monitoring approach and suggested development of bioanalytical screening and predictive modeling tools to improve assessment of the presence of CECs and their potential risk to the environment.

Since 2009 the State Water Board in concert with several Regional Water Quality Control Boards (hereafter collectively referred to as Water Boards) conducted several activities to address CECs at the regional and statewide level. This involved some activities based on recommendations contained in the 2012 Panel report such as use of the risk-based framework to prioritize CECs for monitoring, which led to initiating CEC monitoring in wastewater effluent, stormwater runoff, groundwater, drinking water, and surface water through a variety of programs, permits, and special studies. Table 1.1 includes a summary of 2012 Panel recommendations with Water Boards' activities to implement those recommendations. A detailed summary of these and other CEC activities is available on the State Water Board's CECs Program website at Water Boards CEC Activities Timeline. Many of the projects that have been implemented to date are part of a long-term commitment to characterizing CECs at the regional and statewide level. In addition to CEC monitoring, Water Boards staff took the 2012 Panel recommendations and created a CEC Initiative to take a more holistic approach to monitoring and management of CECs and to be more proactive about addressing CECs in the state.

The CEC Initiative has three phases: compile existing data, knowledge, and resources; improve coordination among State and Regional Water Boards, interagency partners, and stakeholders; and develop and implement a statewide CEC management strategy. Water Boards staff made significant progress towards the first and second phase of the CEC Initiative but did not have dedicated resources to develop CEC management. In June 2020, the Governor approved a budget change proposal to support the state's goals for water resilience in the face of climate change, including addressing threats to water quality due to CECs. With these resources, the State Water Board created a new CEC Program that will continue and build on the work of the CEC Initiative. The CEC Program is in development and some of the core components of the program include: the collection and use of high-quality data, information, and research to improve knowledge and understanding of CECs in California's waters and to support informed, transparent management decisions; identifying and implementing novel approaches to water quality management to move towards a new paradigm of proactive water quality management using a strategic, flexible, and timely approach; interagency coordination with partners such as sister agencies within California Environmental Protection Agency, California Natural Resources Agency, and U.S. Environmental Protection Agency; and conducting education and outreach. CEC Program staff intend to continue to develop the foundation of the program, including by developing a CEC Strategy that will outline program goals and actions for the core components of the program. CEC Program staff will incorporate the recommendations of this 2022 Panel and past Panels in the CEC Strategy. CEC Program staff will periodically update the CEC Strategy. As the program currently only has two full-time staff, they will need to prioritize actions that will have the greatest impact on CEC management on an ongoing basis and expand efforts when the program has additional resources.

**Table 1.1 Activities by the Water Boards related to the implementation of the 2012 Panel recommendations on constituents of emerging concern (CECs).**

| **2012 Recommendation:** Adopt a risk-based screening framework to evaluate CECs and prioritize monitoring | |
|---|---|
| **Water Boards Activity** | **Notes** |
| Development of a CEC Monitoring Dashboard that summarized data for the 16 CECs recommended for monitoring by the 2012 Panel. A dataset was downloaded from California Environmental Data Exchange Network (CEDEN) for samples collected between 1993 and 2016. | This project created a static dataset that has been updated by the data synthesis project described below. The link to this dashboard is no longer available but a new dashboard was developed as part of the 2022 Panel efforts and is available at https://www.waterboards.ca.gov/water_issues/programs/cec/index.html |
| Implementation of data synthesis project whereby available CEC monitoring results in multiple statewide databases were compiled and evaluated against risk-based screening levels (Sutton et al. 2022). Note that this dataset was evaluated in further detail as part of the 2022 Panel report. | This project created a comprehensive dataset and resulted in code that can be managed by the State Water Board to continually update the CEC dataset as new data are submitted or to capture additional information that was not included in the original project. The project also resulted in a summary report to synthesize CEC data using a risk-based screening approach to inform monitoring and management priorities (Sutton et al. 2022). |

| **2012 Recommendation:** Implement an adaptive, four-phased monitoring approach (i.e., planning, data collection, interpretation, and action to minimize impacts) to evaluate the presence of CECs in California | |
|---|---|
| Development of CECs monitoring in aquatic ecosystems quality assurance and quality control guidance (Dodder et al. 2015). | This document describes available quality assurance and quality control guidance for generating a Quality Assurance Project Plan for CEC monitoring. |

| **2012 Recommendation:** Implement an adaptive, four-phased monitoring approach (i.e., planning, data collection, interpretation, and action to minimize impacts) to evaluate the presence of CECs in California | |
|---|---|
| Development of CECs in aquatic ecosystems pilot study guidance to translate the Panel's recommendations into guidance and, where applicable, requirements at a sufficient level of specificity and detail to direct and incorporate into local, regional and/or statewide workplans for future monitoring (Dodder et al. 2015). | This document identified relevant water quality monitoring programs that could consider using the guidance such as the Surface Water Ambient Monitoring Program (SWAMP), Department of Pesticide Regulation, the San Francisco Bay Regional Monitoring Program, the Southern California Bight Regional Monitoring Program, the Bay Area Stormwater Management Agencies Association, the Southern California Stormwater Monitoring Coalition, and other monitoring efforts. |
| Development of a Statewide Pilot Monitoring Plan. The intent of the pilot study monitoring plan was to implement a coordinated approach to evaluating status and trends of CECs throughout the State, and included the use of targeted chemistry, in vitro bioassays, and toxicity monitoring methods (OIMA 2016). | This plan envisioned monitoring for the 16 priority CECs identified by the 2012 Panel. Monitoring locations were identified in Southern California, the Sacramento Delta, Central Valley, and San Francisco Bay. However, implementation of the plan was voluntary, and few participants fully implemented the plan. |
| The North Coast Regional Water Quality Control Board implemented the Statewide Pilot Monitoring Plan in the Russian River watershed (Maruya et al. 2018). | This study was implemented as a direct outcome of the 2012 Panel recommendations, though several other studies were conducted that incorporated elements of the proposed monitoring approach. However, several water quality monitoring programs incorporated aspects of the 2015 CEC monitoring guidance into their studies (San Francisco Estuary Institute 2017; SCCWRP 2018; Maruya et al. 2016). |

| 2012 Recommendation: Conduct research to further knowledge in key areas | |
|---|---|
| Implementation of a project to develop applications for using bioanalytical techniques for monitoring CECs in recycled water (SCCWRP 2014). | This project provided necessary guidance for Water Boards to transition from recommendation to application of CECs monitoring using bioanalytical techniques. |
| Completion of a bioanalytical guidance document and implementation of the guidance (National Water Research Institute 2020). | This project supported the development of commercially available in vitro bioassays for quantification of estrogenic and dioxin-like chemicals in water recycling and reuse but it also supports the availability of analytical methods for CEC monitoring in ambient ecosystems. |
| Further development of bioanalytical screening tools through development of standard operating procedures. | This grant is currently in progress and was developed for the purpose of creating an in vitro bioassay (IVB) toolbox for a variety of ecological and human health endpoints to screen for bioactivity associated with exposure to a wide range of chemicals found in ambient and recycled water using a multi-stage development process. |

## 1.2 Science Advisory Panel

In 2020, the State Water Board and the Ocean Protection Council (OPC) re-convened the Aquatic Ecosystems CEC Science Advisory Panel II (2022 Panel) to provide additional support to the CEC Program. Nominated and vetted through a stakeholder advisory committee represented by the discharger, non-governmental organization (NGO), regulator, and resource communities, the Panel was established in October of 2020 and included seven international experts in the fields of chemistry, biochemistry, toxicology, epidemiology, coastal and marine science, risk assessment, and engineering:

- Dr. Paul Anderson, Independent Consultant
- Dr. Nancy Denslow, University of Florida
- Dr. Jörg E. Drewes, Technical University of Munich, Germany *(Chair)*
- Dr. Derek Muir, Environment and Climate Change, Canada
- Dr. Adam Olivieri, EOA, Inc.
- Dr. Daniel Schlenk, University of California-Riverside

- Dr. Shane Snyder, Nanyang Technological University, Singapore

A brief biography of each panel member and stakeholder advisor is provided in Appendix A. Due to restrictions during the COVID pandemic, the Panel held two in-person meetings and numerous virtual meetings. Some meetings included the opportunity for stakeholder input in clarifying their charge, exchange of information, and dialog with the Panel, and this input was considered in the Panel's recommendations.

## 1.3 Charge Questions

The Panel was provided with six specific charge questions, but was generally asked to review the occurrence, relevance, and quantification of CECs in fresh, estuarine, and oceanic water bodies of California with the goal to provide recommendations for development of a monitoring program for CECs in fresh, estuarine, and oceanic water bodies of California.

1. Which classes of CECs, including those with data gaps, have the potential to adversely impact marine, estuarine and freshwater wildlife, ecosystems, and beneficial uses in marine, estuarine and freshwater environments?
    a. Who are the leaders in the academic field for each of these classes of CECs?
    b. What are the applicable monitoring methods and reporting limits for these classes of CECs?
2. Update the risk prioritization framework developed in the 2012 Panel report (entitled Monitoring Strategies for Chemicals of Emerging Concern (CECs) in California's Aquatic Ecosystems: Recommendations of a Science Advisory Panel) to address classes of chemicals, structurally-related chemicals that may not be within the same class, and data-poor chemical classes (e.g., where there is either no monitoring trigger level or environmental concentration or predicted no-effect concentration).
3. What are the sources, pathways, and rate of inputs leading to the presence of classes of CECs in the marine, estuarine and freshwater ecosystems?
4. Considering the physical, chemical, and biological processes that affect the transport and fate of classes of CECs, what matrices (i.e., tissue, sediment, ambient water, and wastewater) should be screened in each of the three following ecosystems: marine, estuarine and freshwater?
5. What are the most important known and unknown biological effects for specific or classes of CECs and what approaches should be used to assess biological

effects of classes of CECs to sentinel species in marine, estuarine and freshwater ecosystems?

6. How can state management agencies better address classes of CECs in the environment through implementation of the risk prioritization framework? Specifically, how can the State Water Board better address CECs?

Note: Inland freshwater systems refer to surface waters, including streams, rivers, lakes and reservoirs. Coastal aquatic systems are the territorial marine waters of the State as defined by California law, i.e., those extending up to three miles offshore. This question also refers to releases outside three miles that impact state waters or any ground and surface waters (fresh, brackish, or saline) within state boundaries that are hydrologically connected to the coastal ocean.

These charge questions are addressed in the following chapters of this report. In summary, the Panel's overall approach to the charge questions can be summarized as follows.

1. Which classes of CECs, including those with data gaps, have the potential to adversely impact marine, estuarine and freshwater wildlife, ecosystems, and beneficial uses in marine, estuarine and freshwater environments? Identification of CECs, or classes of CECs, that have the potential to adversely affect California's aquatic ecosystems and their beneficial uses depends upon developing and implementing a monitoring program based on robust occurrence data. The range of components of such a program are described in Chapters 2 through 8 of this report. Implementing all of those components was beyond the resources and timeframe available to this Panel. Therefore, the Panel was unable to answer several of the specific questions posed by this charge question. However, once State Water Board Staff implement the monitoring program, the specific elements posed by this charge question will be able to be answered.

2. *Update the risk prioritization framework developed in the 2012 Panel report (entitled Monitoring Strategies for Chemicals of Emerging Concern (CECs) in California's Aquatic Ecosystems: Recommendations of a Science Advisory Panel) to address classes of chemicals, structurally-related chemicals that may not be within the same class, and data-poor chemical classes (e.g., where there is either no monitoring trigger level or environmental concentration or predicted no-effect concentration).* Chapters 5 and 6 present an updated risk prioritization framework originally developed in the 2012 Panel report. Chapters 3, 7 and 8 describe approaches the State Water Board may wish to adopt to address chemicals and chemical classes that are data poor (e.g., by non-target analysis, bioanalytical methods, effects-based analysis, more holistic monitoring

approaches that do not rely on monitoring trigger levels and reliable occurrence data).

3. What are the sources, pathways, and rate of inputs leading to the presence of classes of CECs in the marine, estuarine and freshwater ecosystems? The range of sources and pathways of CECs to aquatic environments was presented in the 2012 Panel report and is briefly summarized in Chapter 1 (Introduction) of this report. The range of sources and pathways remains essentially the same as described a decade ago.

4. Considering the physical, chemical, and biological processes that affect the transport and fate of classes of CECs, what matrices (i.e., tissue, sediment, ambient water, and wastewater) should be screened in each of the three following ecosystems: marine, estuarine and freshwater? As described in Chapters 5 and 6, all matrices should be screened in all three ecosystems. However, all CECs may not need to be screened in all matrices. For example, screening of tissue samples can likely be limited to bioaccumulative and persistent CECs (see Chapter 6.3 and Appendix J). Given the level of effort expended by the Panel to refine the State Water Board dataset, the Panel was only able to apply the monitoring framework to ambient water and using few example CECs in the freshwater, marine and estuarine ecosystems (see Chapter 6.2). Once the State Water Board dataset if fully refined, State Water Board staff will have to screen CECs by apply the monitoring prioritization framework to all matrices in all ecosystems that have available data.

5. What are the most important known and unknown biological effects for specific or classes of CECs and what approaches should be used to assess biological effects of classes of CECs to sentinel species in marine, estuarine and freshwater ecosystems? The Panel reviewed toxicological effects information compiled in a range of readily available databases for all CECs in ambient water in the State Water Board dataset to develop conservative monitoring trigger levels (MTLs) to use in the CEC monitoring prioritization (see Chapter 4, Appendices D and H). As described in the report (see Chapter 4.1), the most sensitive effect reported in the literature was selected to develop conservative MTLs, but that does not necessarily indicate that effect is the most important or relevant effect in ambient water. Identifying the most important effect and sentinel species to monitor requires thorough review of the toxicological literature. This task was beyond the scope of this Panel given the large number of CECs in the State Water Board dataset. Additionally, because the CECs in the State Water Board dataset do not encompass the universe of CECs, in Chapters 3 and 8 the Panel recommends that other databases and sources of information about CECs

be used to identify “new” CECs that may need to be included for monitoring in California (see also Appendix E for a list of potential “new” CECs).

6. How can state management agencies better address classes of CECs in the environment through implementation of the risk prioritization framework? Specifically, how can the State Water Board better address CECs?The Panel developed several recommendations as to how the State Water Board can better address CECs. Those methods include the expanded risk-based prioritization framework described in Chapters 5 and 6, improvements to the current occurrence data compilation and management process described in Chapters 7.2 and 8, incorporating a range of non-traditional assessment methods (e.g., non-target analysis, bioanalytical methods, effects-based analysis) described in Chapter 3 and 7.3, and a recommendation to consider including more holistic monitoring approaches as described in Chapters 7.3 and 8.

## 1.4 The Panel’s Approach

The 2022 Panel was tasked to review the occurrence, relevance, and quantification of CECs with a main focus on ambient surface fresh, marine, and estuarine water ecosystems with the goal to provide recommendations for development of a monitoring program of CECs in fresh, estuarine and oceanic water bodies of California. As one source of CEC occurrence data, the Panel considered the dataset of organic chemicals assembled by the Aquatic Science Center (ASC) for the State Water Board augmented (Sutton et al. 2022) by additional data from California. This dataset covered a period from 2005 to 2022 and also included information on chemicals in sediment and biota. The CEC dataset is described in more detail in Chapter 2.1 of this report. Over 420 chemicals in 11 classes with measured values in fresh, estuarine and marine waters were evaluated individually by the Panel. Broad classes defined by similar chemical structures (e.g., bisphenols), and/or function or purpose in society (e.g., pharmaceuticals) were considered. Building upon this dataset, the Panel established a quality assurance workflow for CEC monitoring data and a risk-based screening framework as illustrated in Figure 1.2. The Panel also used additional multimedia-occurrence data considering other state, national and international sources reporting on CECs not currently included in California’s ongoing previous or existing monitoring programs. In addition, the Panel considered additional sources on toxicity to sensitive species and assembled toxicity threshold values for these CECs. Applying this framework will result in a preliminary monitoring prioritization, a refined monitoring prioritization, and a final recommended monitoring list or programs.

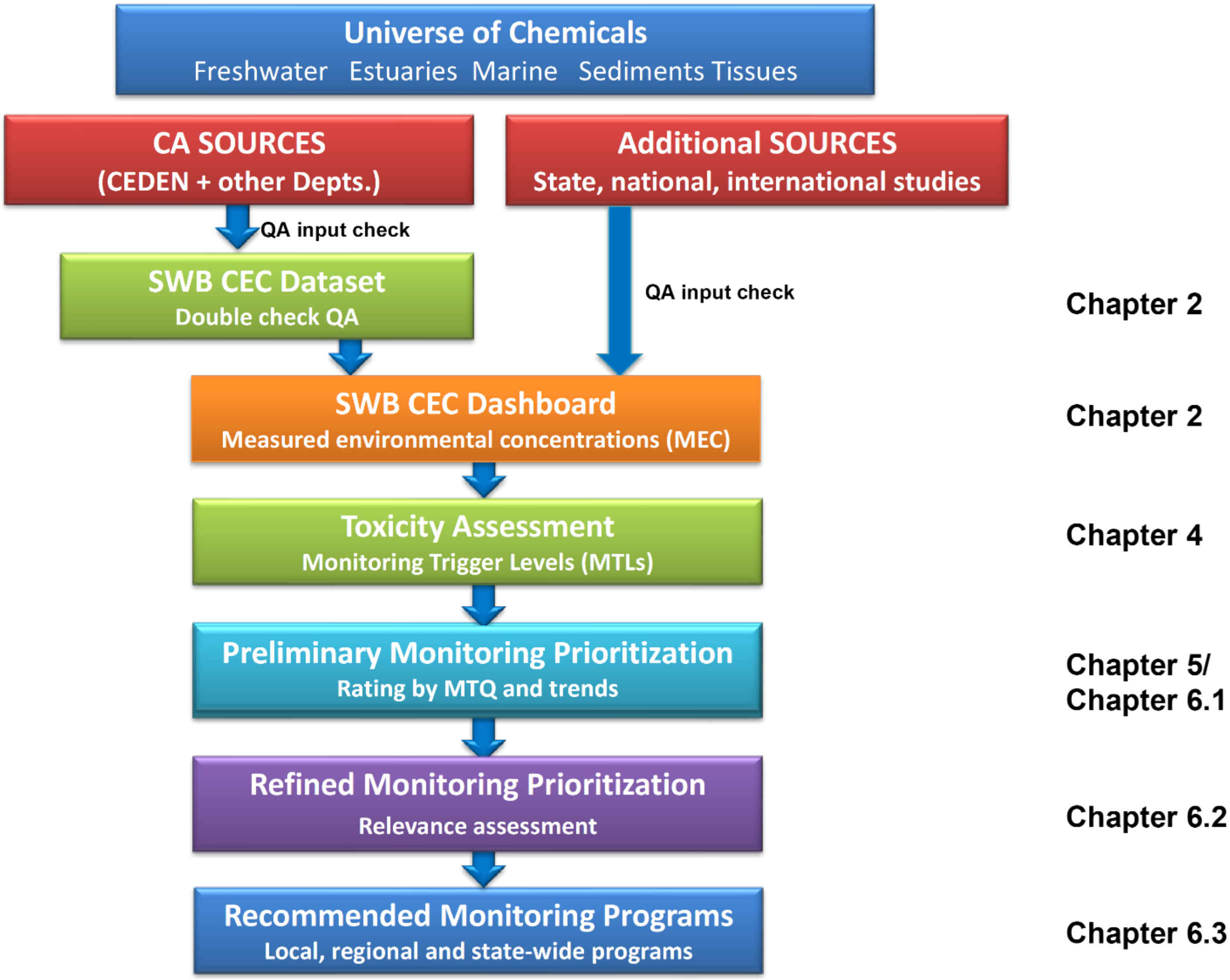


**Figure 1.2. The Panel's approach and workflow to identify relevant constituents of emerging concern (CECs) for monitoring in the aquatic environment and indications in which chapters of this report additional information is provided.**

Given the substantial time associated with the cleanup of the CEC dataset, the Panel refocused on demonstrating a "proof of concept" for an updated and expanded risk- and occurrence-based monitoring prioritization framework, providing the Water Boards with a model, and a road map to use when developing the monitoring prioritization and broader implementation, including dataset updates, as part of the statewide CEC Program. In essence, the overall recommendation for the State Water Board CEC Program is to complement the continuing risk-based monitoring approach with temporal and spatial evaluations, improve the quality of data reported to the State Water Board, regularly update the monitoring trigger levels (MTLs) as new CEC monitoring and toxicology information become available, develop a pilot biomonitoring program focused on early identification of effects in ambient waters, work with a future Ambient Ecosystems CEC Advisory Panel or an equivalent process for expert review, and ultimately update existing policy and monitoring requirements to update the State's approach to CEC monitoring and management, and to guide a state-wide CEC monitoring program for receiving waters. This report provides the results from the Panel's deliberations.

# 2. Assessment of the State Water board CEC Dataset

To assess sources, pathways, and rate of inputs leading to the presence of classes of CECs in the fresh, estuarine, and marine water ecosystems, the Panel utilized and expanded the CEC dataset provided by the State Water Board (in response to Charge Question #3). Considering the wide range of physico-chemical properties of these CECs, the Panel considered different matrices (i.e., dissolved and total concentrations in ambient fresh, wastewater, estuarine and marine water, tissues and sediments) to assess the relevance of specific CECs for the aquatic environment (in response to Charge Question #4).

## 2.1 High-Level Assessment of State Water Board Dataset

### 2.1.1 Compilation of datasets and refinements

Occurrence data for CECs recorded in the State Water Board dataset and published in the peer-reviewed literature were assembled for the ASC report (Sutton et al 2022). A full description of the occurrence dataset and the challenges associated with making it amenable for use is provided in Section 2.3 of the ASC report. Here we provide an overview of the issues encountered in refining the State Water Board dataset to enable presentation on a CEC Dashboard and for the subsequent risk-based assessment and prioritization of CECs.

#### *CEC occurrence data from California State Water Board dataset*

ASC compiled a list of CECs using many resources, including "public databases of environmental data; analyte lists from available standardized or commercially available analytical methods; presence within class-based lists compiled by other agencies, such as the California Biomonitoring list of designated chemicals (https://biomonitoring.ca.gov/chemicals/designated-chemicals); and recent reviews of CEC classes published in scientific journals". This list was then used to extract monitoring records of these chemical analytes in the dataset for California's ambient aquatic ecosystems listed in Table 2.1. The extracted data formed the core of the risk-based monitoring prioritization for the assessment of CECs in aquatic media.

Further details on the data mining are provided in Appendix B, which includes a description of the dataset fields, use of SQL, file formats, etc.

Each record in the dataset included core data such as Project name, Station, Location, Sample Date, Sample Type (field, blank, duplicate, etc.), Site Type (e.g., Bays and Harbors, rivers/streams), Parameter (chemical name), Result (or non-detect), Units (original units and a separate field was added to convert results to a standard unit, µg/L or parts per billion (ppb)), MDL/RL (method detection limit / reporting limit), Sample Matrix (may be inferred from data source), compound class, and LabAgency. In total, the dataset included 59 fields for each record. A "record" represents the measurement of an individual CEC. Typically, a single sample would be analyzed for multiple CECs, and each CEC would have its own unique record.

The dataset was provided by ASC to the State Water Board as a draft working product to inform the parallel activities of the Panel. State Water Board staff conducted data processing using Python, provided additional geospatial metadata, and removed records not suitable for use (e.g., concentrations reported without units, passive sampler results, QA samples such as measurements of recovery standards). Full details of the clean-up steps are provided in Appendix B2. Key characteristics of the final CEC dataset are summarized in Table 2.2.

An important element of the State Water Board revision was the addition of information about sample collection sites to classify the records into fresh, estuarine, and marine so that risk-based prioritization could be conducted separately for each of these types of ecosystems. While records for surface water, sediment, tissues of biota, wastewater influent/effluent, and stormwater were compiled in the occurrence dataset, the Panel focused its assessment on the surface water records in fresh, estuarine, and marine settings.

**Table 2.1. Sources of occurrence data for constituents of emerging concern (CECs) compiled in the State Water board dataset.**

| Database Name | Organization |
|---|---|
| CEDEN (http://www.ceden.org/) | State Water Board |
| Water Quality Portal (https://www.waterqualitydata.us/) | NWQMC (EPA WQX, USGS NWIS) |
| SDWIS, California EDT (https://www.waterboards.ca.gov/drinking_water/certlic/drinkingwater/publicwatersystems.html) | State Water Board |
| CIWQS | State Water Board |

| | |
|---|---|
| (https://www.waterboards.ca.gov/water_issues/programs/ciwqs/) | |
| GeoTracker – PFAS Only (https://geotracker.waterboards.ca.gov/map/pfas_map) | State Water Board |

An important element of the State Water Board revision was the addition of information about sample collection sites to classify the records into fresh, estuarine, and marine so that risk-based prioritization could be conducted separately for each of these types of ecosystems. While records for surface water, sediment, tissues of biota, wastewater influent/effluent, and stormwater were compiled in the occurrence dataset, the Panel focused its assessment on the surface water records in fresh, estuarine, and marine settings.

**Table 2.2. Summary of the entries for constituents of emerging concern (CECs) in the State Water Board dataset.**

| Media | Matrices | Total records | Detected (>0) | Detection frequency (%) | Total analytes |
|---|---|---|---|---|---|
| Surface waters | Estuarine | 8,880 | 1,550 | 17% | 251 |
| Surface waters | Freshwater | 280,653 | 33,561 | 12% | 396 |
| Surface waters | Marine | 21,385 | 6,399 | 30% | 338 |
| Surface waters | Not recorded | 116,193 | 12,818 | 11% | 306 |
| Sediments | Estuarine | 15,871 | 3,002 | 19% | 234 |
| Sediments | Freshwater | 61,245 | 8,508 | 14% | 140 |
| Sediments | Marine | 46,173 | 13,351 | 29% | 268 |
| Sediments | Not recorded | 7,363 | 2,951 | 40% | 142 |
| Stormwater | Location provided | 30,775 | 10,511 | 34% | 138 |
| Stormwater | Location not recorded | 330 | 26 | 7.9% | 29 |
| Effluent/influent | Influent | 17,718 | 3,547 | 20% | 70 |
| Effluent/influent | Effluent | 56,686 | 7,339 | 13% | 321 |

| Media | Matrices | Total records | Detected (>0) | Detection frequency (%) | Total analytes |
|---|---|---|---|---|---|
| Effluent/influent | Biosolids | 1,064 | 108 | 10% | 12 |
| Biota | Estuarine | 3,673 | 2,812 | 77% | 213 |
| Biota | Freshwater | 5,108 | 1,164 | 23% | 120 |
| Biota | Marine | 16,301 | 4,473 | 27% | 96 |
| Biota | Not recorded | 5,399 | 1,768 | 33% | 80 |

Total records for CECs analyzed in surface water ranged from 8,880 in estuarine waters to 280,653 in freshwater. These represented results from 3,622 sampling stations. However, a large proportion of surface water results (27%; 116,193 of 427,111 records) were listed as “not recorded” due to lack of information such as latitude/longitude or a description of the site (parameter “Site type”). The sampling years for fresh, estuarine, and marine water ranged from 2005 to 2021 with the largest number of records from 2017 (Appendix C, Figure C.1).

**Table 2.3. Numbers of records reporting concentrations of constituents of emerging concern (CECs) as dissolved or total in the State Water Board dataset. The dissolved result represents filtered samples, while total results are unfiltered. This information was provided under the parameter “FractionName” in the State Water Board CEC dataset.**

| Water type | Fraction | Records |
|---|---|---|
| Fresh | Dissolved | 152,996 |
| Fresh | Total | 99,746 |
| Estuarine | Dissolved | 9,076 |
| Estuarine | Total | 0 |
| Marine | Dissolved | 0 |
| Marine | Total | 21,385 |
| Not recorded | Total | 0 |

Measurement of CECs in estuarine waters involved filtration of the samples while for marine waters, all samples were unfiltered (Table 2.3). For freshwater samples, about 60% of results were reported as dissolved. While dissolved concentrations are regarded as more likely to represent a bioavailable fraction (Anderson et al., 2012), our prioritization process at this time does not give preference to dissolved versus total concentrations (Chapter 5).

Measurements of CECs in sediments constituted the next largest group of results, ranging from 15,871 in estuaries to 61,245 in freshwaters. Site-type information was missing for 5.6% of the sediment entries. Influent, effluent and biosolids from WWTPs were the next largest group of records with 75,468 analyses. The majority of the WWTP records were for effluents. Stormwater records constituted the next largest group (31,105 records). Analyses of biological records constituted the next largest group (25,082 records) with marine biota constituting the majority of records (Table 2.2). Bivalves and fish were major sample matrices in marine and estuarine waters while results for fish predominated in freshwater records.

A total of 423 CECs were reported across all media. These CECs were categorized into eleven classes: Pesticides, pharmaceuticals, alkyl phenols/alkyl phenol ethoxylates (AP/APEs), phthalates, polybrominated diphenyl ethers (PBDEs), brominated flame retardants (BFRs), PFAS, personal care products (PCPs), bisphenols, organophosphate esters (OPEs), and natural toxins (microcystins and marine toxins) (Figure 2.1, Appendix C. Table C.1).

Pharmaceuticals constituted the largest group of individual CECs in freshwater (108) and estuarine waters (83), although only five were reported in marine waters (Figure 2.1). Pesticides were the next largest group ranging from 44 compounds in marine water to 108 in freshwater. PBDEs were the third largest group in water due to reporting for 51 congeners. Highest detection frequencies (DFs) for PBDE in freshwaters were for congeners 15, 28, 47, 49, 99, 100, 119, 140 and 153 (Appendix B, Table C.2). Distributions of the 11 classes of substances in sediments and biota are illustrated in Appendix C, Figure C.2 and summarized in Table C.1.

Two sets of summary data were calculated for each CEC (arithmetic mean, standard deviation, minimum, maximum as well as 25$^{th}$, 50$^{th}$, 75$^{th}$ and 90$^{th}$ percentiles) in surface waters. The first set of summary data (Appendix C, Table C.3) was based on only detected concentrations of a CEC. The second set of summary data was calculated using all the results, including non-detects, where the concentration of a CEC in a non-detect sample was assumed to be a method detection limit (MDL) equal to the median detection limit of all samples of that CEC for that time period (Appendix C, Table C.4). Appendix C, Tables C.5 and C.6 include additional statistics for substitution with the minimum MDL and for detection limits. The 90$^{th}$ percentile was selected as the measured environmental concentration (MEC) when conducting the risk-based monitoring prioritization. The 90$^{th}$ percentile value is inclusive of existing reported concentrations, rather than an interpolated number.

### *Discussion of detection limits*

Across all CECs and surface water sample locations detection frequencies (DFs) for CECs in surface waters ranged from 12% in freshwater to 30% in marine waters (Table 2.2). However, at the level of individual CECs, DFs ranged from 0 to 100% (Appendix C, Tables C.2, C.3, and C.4). **Thus, a significant portion of the monitoring data were non-detects.** Further complicating the process of cleaning up the dataset, detection limits for individual CECs often spanned several orders of magnitude, or were listed as zero or left blank. Substitution of the detection limits by a specific rule such as ½ that value or based on the statistical distribution of reported measured values (Helsel 2010, Antweiler 2015) was impractical given the range of detection limits. Various approaches to substitution of non-detect data were considered by the Panel and the median MDL value was chosen. This substitution was made only for a given analyte and matrix and where at least one result above the detection limit was available.

The effect of substitution of the median MDL on the value of the 90$^{th}$ percentile was greatest for pesticides, pharmaceuticals, and PCPs in freshwater samples where 47% to 80% of 90$^{th}$ percentiles were more than 10-fold higher than the 90$^{th}$ percentile based only on detected concentrations (Appendix C, Table C.2). Substitution of the median MDL lowered the 90$^{th}$ percentile by >10-fold in a more limited number of pesticides (10 of 99 in freshwater; 4 of 43 in estuarine water). Further discussion of the detection limits is provided in Appendix C using three examples: 3,4-dichloroaniline (DCA), erythromycin and 17β-estradiol (17β-ES) in freshwater samples, with Figure C.3 illustrating the distribution of detection limits compared to the median detection limit. These three were selected because they represent a wide range of detection frequencies and detection limits.

Substitution of the median MDLs reduced the degree of censoring of the data. Censoring refers to data with a high proportion of values stated as below a specific value, such as a detection or reporting limit (e.g., “less-than” values). However, substitution clearly introduces uncertainty about the true range of concentrations in ambient waters. In the case of DCA, which had a 69% DF, the 90$^{th}$ percentile was reduced < 2-fold, from 0.20 to 0.12 μg/L by this substitution. For erythromycin and 17β-ES, which had DFs of 2.7% and 1.4%, respectively, the substitution increased the 90$^{th}$ percentiles over 10-fold. For erythromycin the 90$^{th}$ percentile was 10 μg/L compared to 0.22 μg/L based on three measured values. For E2, the 90$^{th}$ percentile was 0.8 μg/L compared to 0.001 μg/L based on a single measured value. These cases illustrate that no substitution method works well for highly censored data (i.e., < detection limits), as has been demonstrated for smaller more focused contaminant datasets (Antweiler 2015). In the future, a more robust data entry process is needed to screen out detection limits that are orders of magnitude higher than the median MDL or some other concentration determined to be an appropriate target MDL. Guidance is also needed for monitoring programs to achieve lowest practical detection limits to avoid, as much as possible, a high proportion of “less than” values.

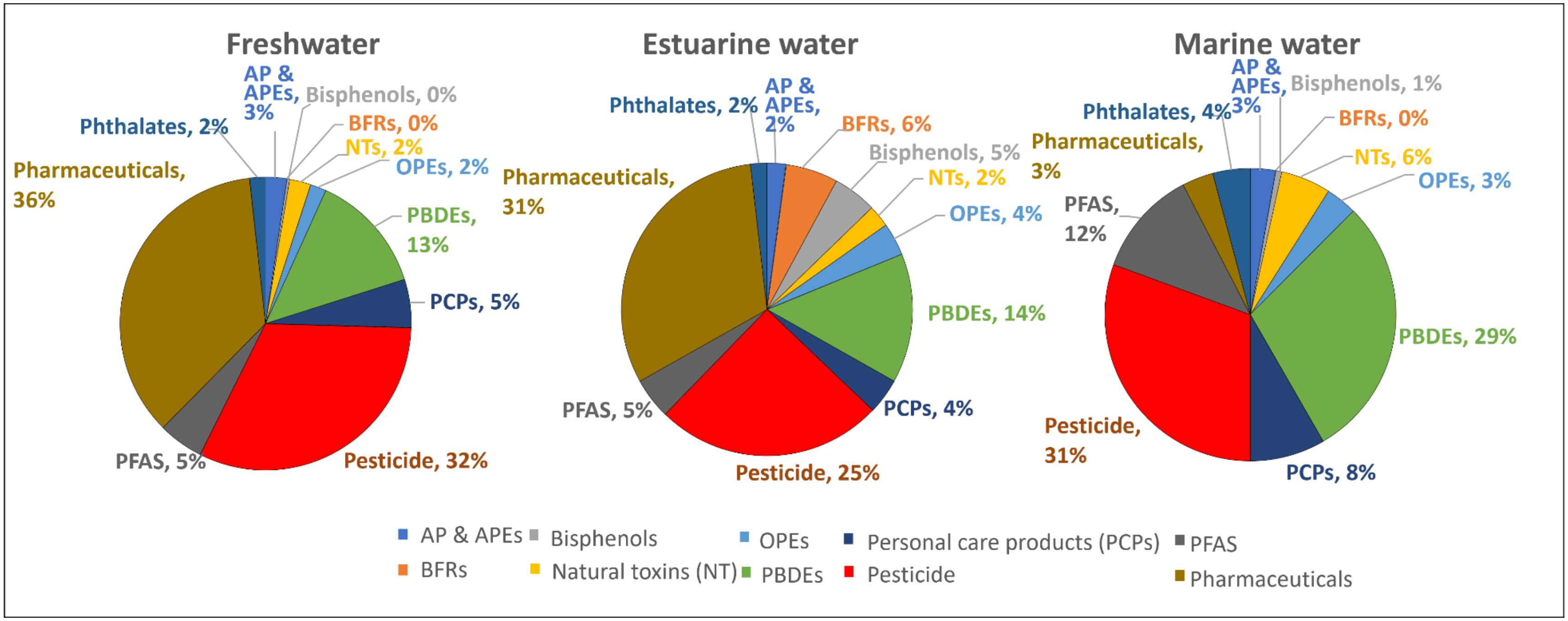


**Figure 2.1. Distribution of various classes of constituents of emerging concern (CECs) in surface waters based on the State Water Board dataset. Alkylphenols and alkylphenol ethoxylates are AP & APEs, brominated flame retardants are BFRs, natural toxins are NT, organophosphate esters are OPEs, polybrominated diphenyl ethers are PBDEs, personal care products are PCPs, and per- and polyfluorinated alkyl substances are PFAS.**

## 2.1.2 State Water Board CEC Dashboard visualization

The State Water Board intends the collected CEC data to be useful, accessible, and interoperable; to inform all stakeholders about water quality and potential risks in water bodies of interest; and to fundamentally support the mission of the State Water Board's CEC Program. Consistent with the goal to enhance its data culture, the State Water Board invested in a data tool kit to support the State Water Board staff use of any software program to access, manipulate, analyze, and interactively visualize data and to create sophisticated data-based reports and applications. For the purpose of the Panel, *Tableau* (Tableau Software, LLC) was selected as the initial platform that provides a simple interface for interactive geospatial evaluation and allows for advanced data analysis on large or multiple datasets with simple interfaces and dashboards. While *Tableau* was selected, it is one of many options that are available to the State Water Board staff. Further, the underlying dataset is intended to be open access and available for import to other such tools.

The initial State Water Board dataset was compiled as part of the ASC Data Synthesis Project (Sutton et al. 2022) and further refined by the State Water Board working with the Panel in accordance with the methods described in Chapter 2.1.1. The CEC dataset was saved as a MS Excel™ Workbook and published on the State Water Board *Tableau* server for access by the Panel. The *Tableau* workbook was organized with specific attributes such that data could be filtered and visualized using the following user options:

- Results including Sample Result Detected and Sample Result Not Detected[1];
- Site type of freshwater, estuarine, or marine;
- Sample matrix of benthic, biota, bird, mammal, sediment, or water;
- Analyte class of AP/APEs, BFR, Bisphenols, NTs, OPEs, PBBs, PBDEs, Personal Care Products, Pesticides, Pharmaceuticals; and
- Analytes of all CECs included in the State Water Board dataset.

Data filters can be applied by each user and the data display was designed to illustrate results in a time series using an embedded chart and geographically on a map of California. Data can be displayed using a color scale to provide a visual evaluation of

[1] In records where the result was 'non-detect', the method detection limit is shown; in cases where the result was 'non-detect' AND where there was no method detection limit reported, a median method detection limit for the relevant compound in the relevant matrix and site type was used. Chemicals lacking any detected values were not included in the risk assessment and prioritization. For more information on the detection limit see Appendix C and Chapter 2.1.1.

the range of concentrations observed throughout the state spatially. However, for Figures 2.2 to 2.7 we chose to show the geographic scope of the non-detect and detectable results and display the concentrations in a temporal trend insert on the map.

Figures 2.2 to 2.7 illustrate how data filters can be used to visualize non-detected and detected results by matrix and substance class spatially on a map of California. The following examples illustrate the results for the freshwater matrix. Illustrations for select example CECs with a preliminary high monitoring prioritization along with times series information are presented in Chapter 6.

For the examples below, the data are shown for each sampling location, with separate symbols for detected concentrations and non-detect values. All results are reported as ppb (µg/L or µg/kg) where non-detects have been replaced with the median detection limit or the actual detection limit where available. The summary table in each figure provides additional information on total number of records and total number with a result reported (i.e., > detection limit).

Figure 2.2 displays results for all matrices and compounds in the dataset. The figure indicates a substantial coverage of California in terms of sampling sites. Of the 449,603 records, 79% were reported as non-detect (grey symbols). From an overall perspective, depending on the specific compound, matrix and MDL, the non-detects may be useful for informing a subsequent selection process. The sampling date insert shows that the majority of samples were collected in the period 2010-2018.

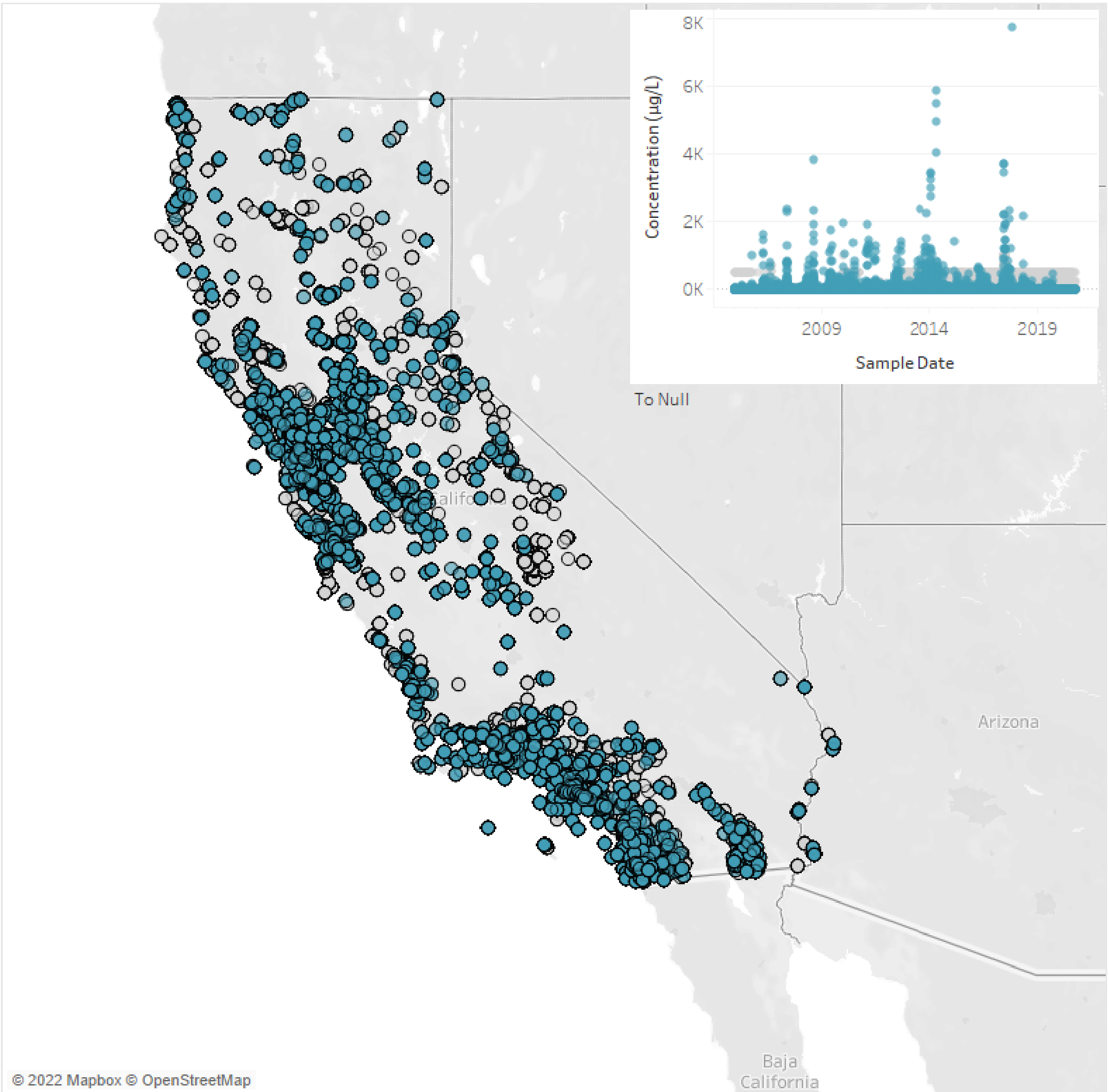


**Figure 2.2. California occurrence data coverage for all matrices and all Constituents of Emerging Concern (CECs) in State Water Board Dataset. Total number of records are 694,817 and 427,111 for all matrices and for water, respectively. Total records above the method detection limits (MDLs) are 113,888 and 54,328 for all matrices and for water, respectively. Teal symbols are detected measurements, grey symbols are non-detect measurements, i.e., below MDLs. Concentrations, in micrograms per liter (ug/L) or micrograms per kg (ug/kg), over time in inset plot. Note that detections do not necessarily imply risk or hazard, nor do non-detects necessarily imply lack of risk or hazard.**

Figure 2.3 displays data for CECs in fresh, estuarine, and marine surface waters analyzed and reported within the State Water Board dataset. Results are shown for up to 423 analytes and 3,622 sampling locations. The majority of data are from sampling conducted in 2013-2018. Roughly 87% of the fresh, estuarine, and marine water records were reported as non-detect (Table 2.1). The prominence of non-detects is also evident from the horizontal grey lines which are indicative of the same detection limits being consistently reported in multiple years. However, 14% of the data could not be used because they were listed as zero (1%) or left blank (13%) and thus lacked information to estimate/interpret an MDL.

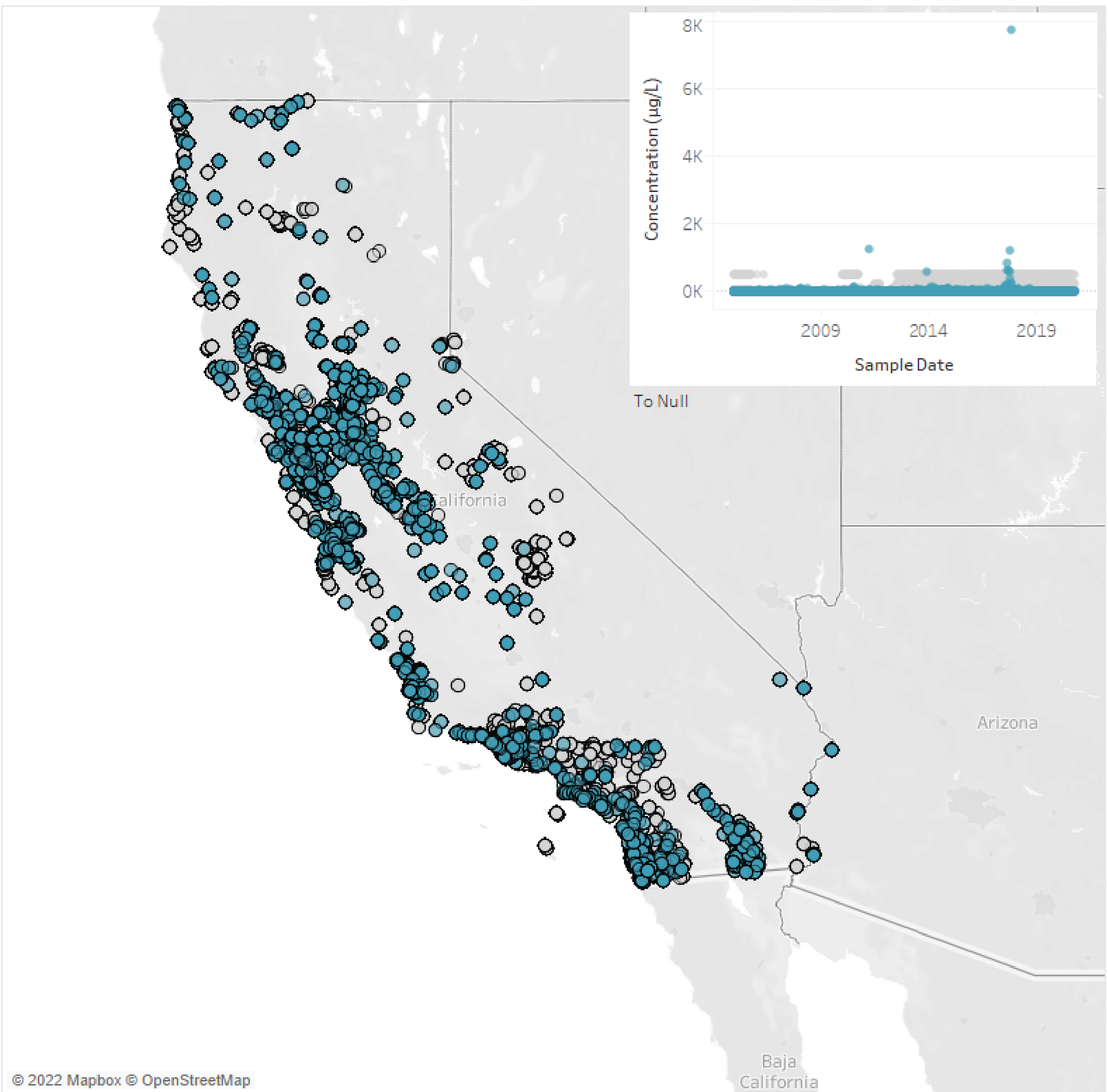


**Figure 2.3. California occurrence data coverage for all Constituents of Emerging Concern (CECs) for all water matrices. Total number of records are 427,111, 280,653, 8,880, and 21,385 for all water, freshwater, estuarine water, and marine water, respectively; numbers above method detection limits (MDLs) are 54,328, 33,561, 1,550, and 6,399, respectively.**

**Teal symbols are detected measurements, grey symbols are non-detect measurements, i.e., below MDLs. Concentrations in micrograms per liter (ug/L) over time in inset plot.**

Figure 2.4 displays all usable CEC data for freshwater records. Approximately 351,000 records were classified as freshwater of which 280,650 were for surface waters. The majority of data are from sampling campaigns conducted in 2009-2018.

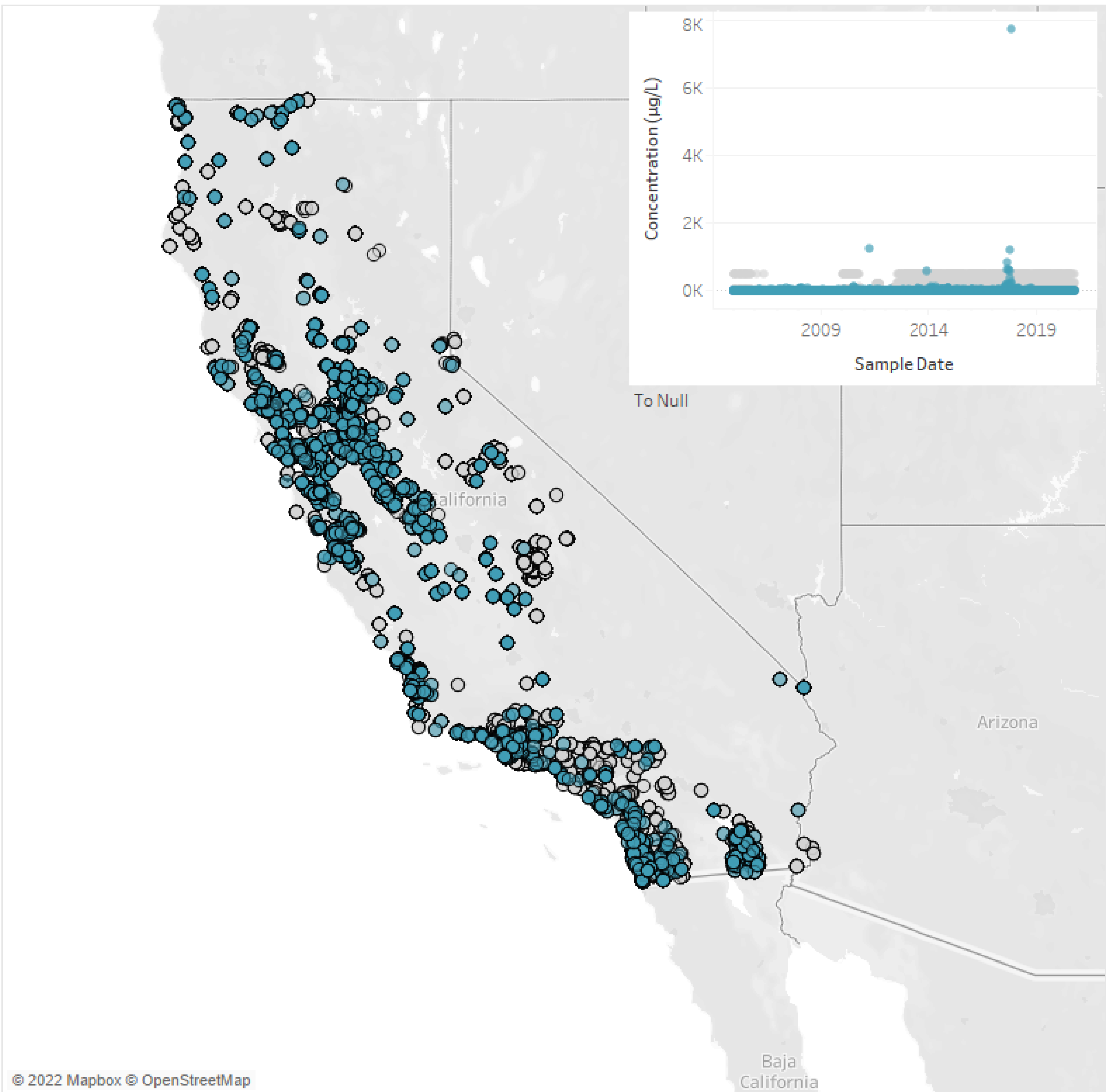


**Figure 2.4. California occurrence data coverage for all Constituents of Emerging Concern (CECs) for all water matrices. Total number of records are 280,653 for 396 analytes, with 35,561 for 338 analytes above method detection limits (MDLs). Teal symbols are detected measurements, grey symbols are non-detect measurements, i.e., below MDLs. Concentrations in micrograms per liter (ug/L) over time in inset plot.**

Figure 2.5 displays results for pesticides in freshwater. There were 280,650 records for pesticides in surface waters based on results for 99 compounds having at least one detection.

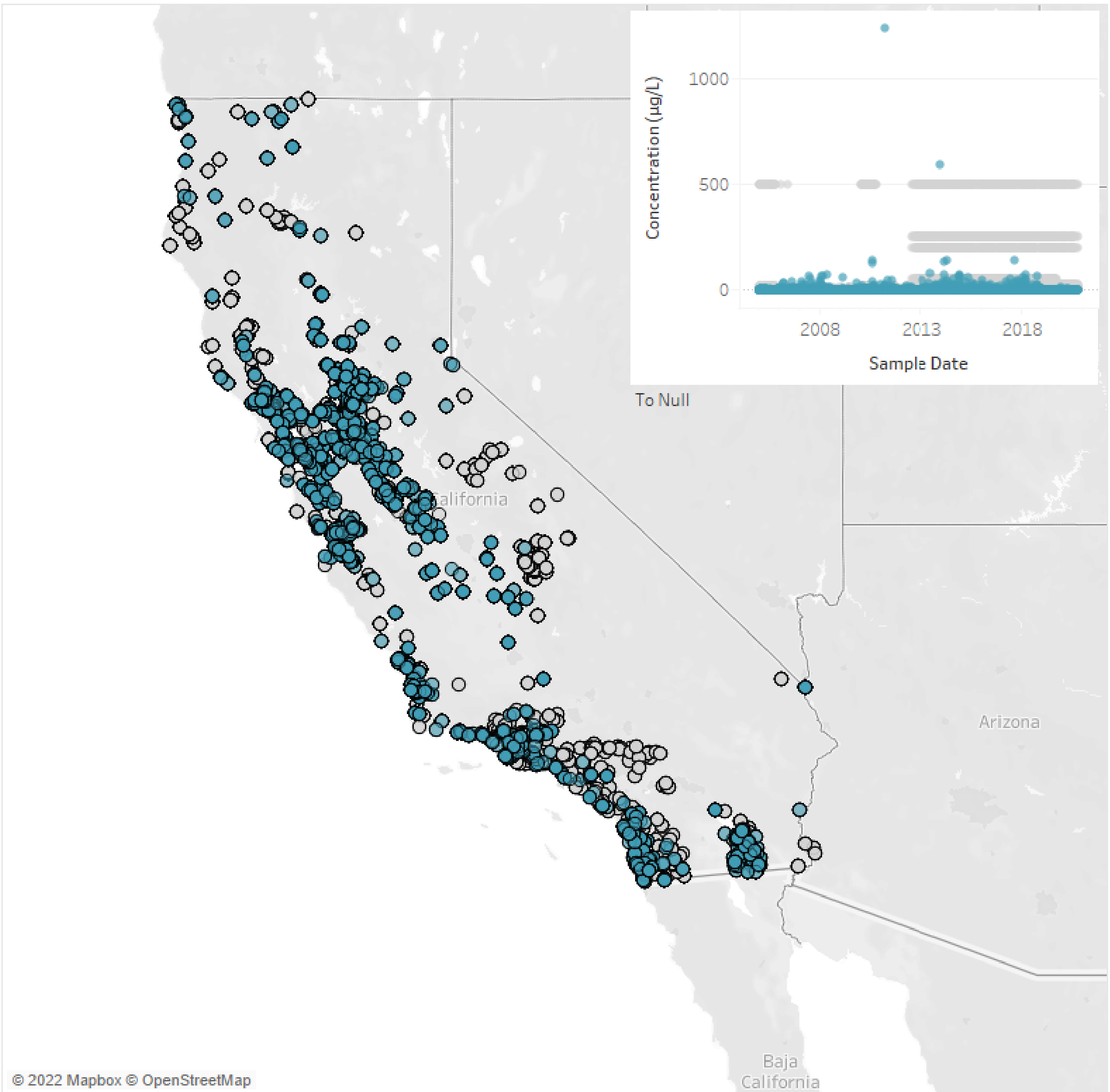


**Figure 2.5. California occurrence data coverage for pesticides in freshwater. Total number of records are 210,264 for 108 analytes, with 30,639 for 99 analytes above method detection limits (MDLs). Teal symbols are detected measurements, grey symbols are non-detect measurements, i.e., below MDLs. Concentrations in micrograms per liter (ug/L) over time in inset plot.**

Figure 2.6 displays results for OPEs in fresh, estuarine, and marine surface water samples. There were 1,172 records based on 12 compounds. The majority of results were from estuarine waters (707).

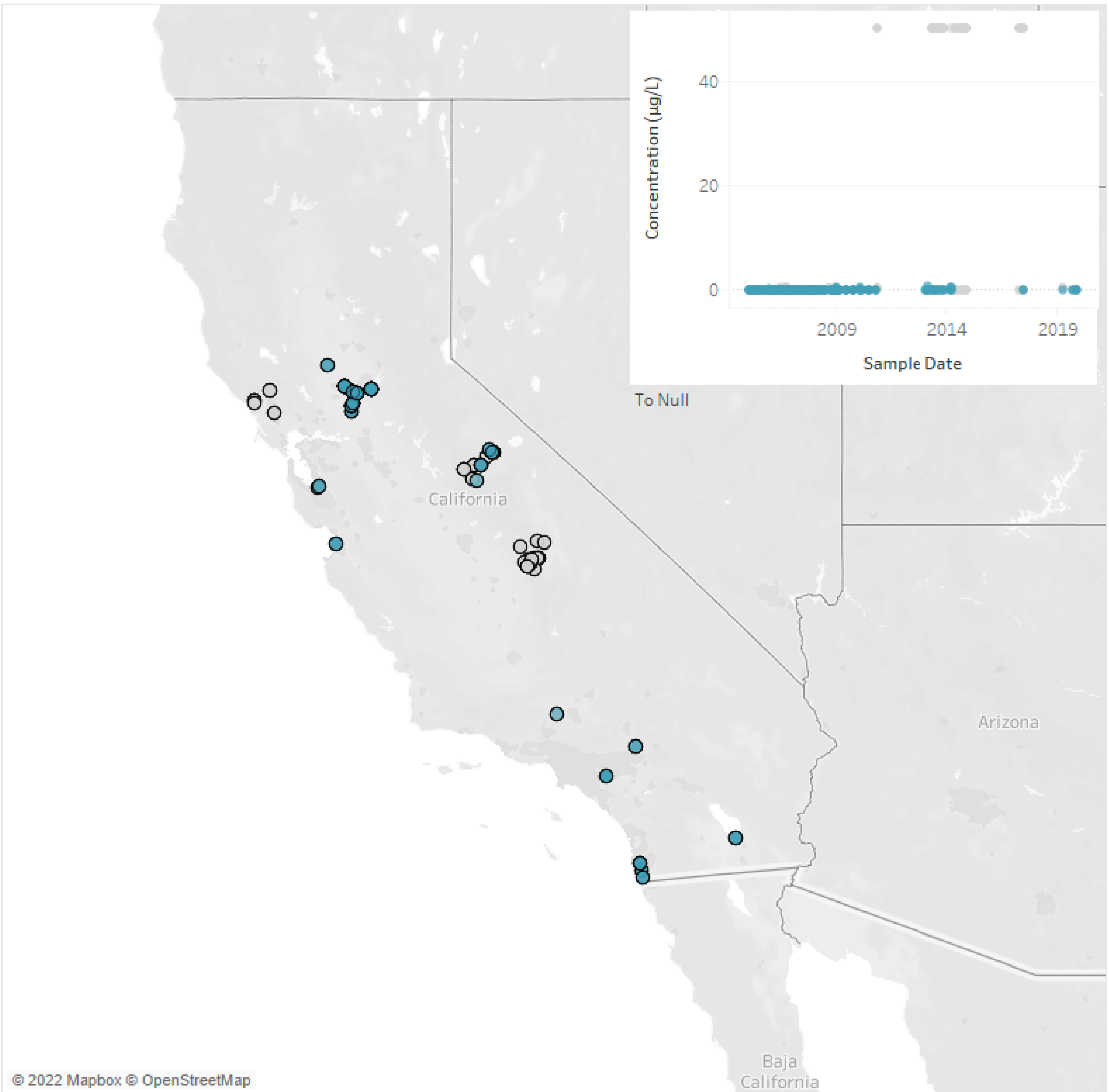


**Figure 2.6. California occurrence data coverage for organophosphate esters (OPEs) in freshwater, estuarine, and marine waters. Total number of records are 441 for freshwater (6 compounds), 707 for estuarine water (12 compounds), and 24 for marine waters (5 compounds; the analogous record count above method detection limits (MDLs) are 249, 407, and 0, respectively. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations in micrograms per liter (ug/L) over time in inset plot.**

Figure 2.7 displays results for PBDEs in marine and estuarine sediments. PBDEs were the major group of CECs analyzed for in marine and estuarine sediments representing 62% of all records. A total of up to 63 PBDE congeners were analyzed for in sediments (up to 47 detected) classified as “marine” or “estuarine” based on 54,500 records. The majority of the results were for tetrabromo PBDE congeners 47 and 49 and pentabromo congeners PBDE 99 and 100. In addition, 21 other BFRs were determined in estuarine, marine, and freshwater sediments.

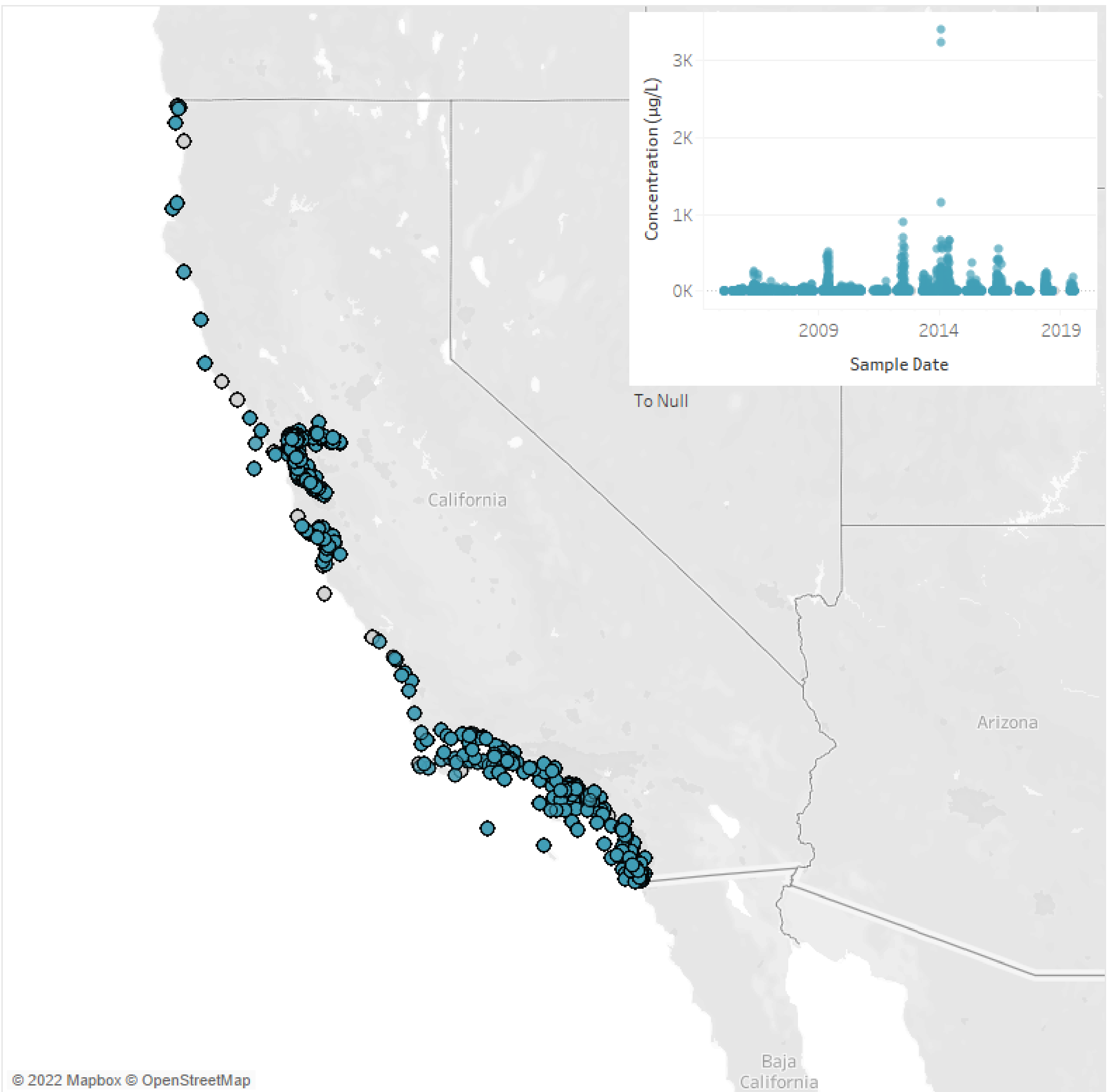


**Figure 2.7. California occurrence data coverage for polybrominated diphenyl ethers (PBDEs) for marine and estuarine sediments. Total number of records are 43,416 for estuarine sediments (47 congeners) and 11,087 for marine sediments (42 congeners); the analogous number above method detection limits (MDLs) are 18,832 and 1,898,**

**respectively. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations in micrograms per kg (ug/kg) or parts per billion (ppb) over time in inset plot.**

## 2.2 Summary

The State Water Board dataset used in this report was assembled in a data synthesis report prepared by ASC (Sutton et al. 2022) and was based on monitoring records for 11 classes of CECs analyzed from 2005 to 2022 in California's ambient aquatic ecosystems. The majority of the records were for surface waters (61%); sediment, and influents/effluents constitute 30%. The Panel focused its assessment on the surface water records in fresh, estuarine, and marine settings. Pesticides and pharmaceuticals constituted the majority of the chemicals analyzed in freshwater and estuarine samples (67 and 61%, respectively). A large number of records were available for surface waters (280,653 in freshwater) and geographic coverage was very good with results from up to 3,622 sampling stations. However, only 12% (freshwater) to 30% (marine waters) of the records reported detectable concentrations. But the detections do not necessarily imply risk or hazard, nor do non-detects necessarily imply lack of risk or hazard. Subsequent chapters put the detects in the context of risk.

There was a substantial amount of CEC data collected since the Panel was last convened. However, since the data came from many different sources with various data quality standards, this not only took a substantial amount of time to try to reconcile the differences, but also highlighted the need for statewide guidance on data quality objectives for CEC monitoring. For example, the lack of the latitude/longitude information for 27% of surface water results severely limited the utility of the data. Further complicating the records, detection limits for individual analytes often spanned several orders of magnitude, were listed as zero, or left blank. This seems to have been due to multiple agencies providing data with different reporting limits. When calculating the MEC (i.e., the 90$^{th}$ percentile) for a CEC, the Panel utilized the available detection limit information and substituted the median CEC-specific detection limit for non-detect samples of that CEC, as long as that CEC was detected in at least one sample. This resulted in 90$^{th}$ percentiles for the substituted datasets being higher than the 90$^{th}$ percentiles based only on reported data for many pesticides and pharmaceuticals. On the other hand, it enabled better use of the available data for highly censored chemicals that had at least some detectable levels. Visualization of the data with *Tableau* enables more detailed evaluation of the data as illustrated in Figures 2.2 to 2.7 including geographic coverage for detects and non-detects, frequency of sampling, and temporal trends in concentrations.

# 3. Other sources for MEC Occurrence data

To inform what CECs should be considered in monitoring programs in California, occurrence data sources beyond the State Water Board dataset, both within the State of California and outside of it, can be used to identify applicable analytical methods and reporting limits for these CECs (in response to Charge Question #1b). In addition to the use of target analyses methods, important known and unknown biological effects for specific or classes of CECs could be assessed using non-targeted analyses (NTA) (in response to Charge Question #5). These approaches need to be critically evaluated to determine how well they assess biological effects of classes of CECs to sentinel species in fresh, estuarine, and marine water ecosystems.

Non-targeted analyses are highly valuable when developing comprehensive programs for identifying potential substances of environmental risk. Non-targeted analyses generally include mass spectrometric techniques, bioassays, and iterative combinations of instrumental and bioanalytical techniques. More broadly, suites of metals and other elements are also part of comprehensive NTA, whereby modern instruments are capable of identifying nearly any atom in the periodic table (i.e., Inductively Coupled Plasma Mass Spectroscopy). Non-targeted analyses also can include surrogate species, such as on-line UV transmission, fluorescence, and total organic carbon.

## 3.1 Background – Expanding the Focus to Other Sources and "New" CECs

Water is especially susceptible to pollution since human activities produce both solid, liquid, and gaseous waste streams that ultimately can enter natural water systems. Everyday new natural and synthetic chemical substances are discovered, many of which ultimately enter the market in a very wide diversity of commercial products. Targeted analyses are limited to substances that have known or suspected occurrence in the environment; however, these analyses measure only a small subset of the chemical substances that can and do occur in the environment. Regulatory requirements are the largest driver of targeted analyses in most environmental scenarios. For instance, both the World Health Organization (WHO) and the U.S. EPA provide guidance and/or standards for approximately 100 parameters for public water systems. However, over 199 million chemical substances were registered by Chemical Abstract Services (CAS) as of August 2022 (https://www.cas.org/cas-data/cas-registry) and an additional 15,000 have been estimated to be added each day. These numbers are even more confounded by the nearly infinite amount of transformation products that can, and will, form during certain water treatment processes or processes that occur naturally in receiving waters. Therefore, many chemical substances that may have a detrimental impact to the environment and/or human health may not be discovered until deleterious effects are observed. For these reasons, the Panel decided to consider data from sources beyond measured environmental concentrations within the State of California (Chapter 3.2) and has provided refined recommendations regarding the use of instrumental and bioassay non-targeted analyses (Chapter 3.3).

## 3.2 Additional Information Considered

The Panel sought to include other chemicals that were not reported to the State Water Board statewide dataset. The first source was a literature survey prepared for the ASC report (Sutton et al. 2022) which included data for chemicals in surface waters, sediments, stormwater, wastewaters and biota in California from the peer-reviewed literature. From those data 25 compounds were identified that were not in the State Water Board CEC dataset for surface waters. Only substances with detected concentrations were included. Appendix E lists these “new CECs” along with data sources.

The Panel also conducted a search of studies utilizing NTA to identify a broader range of CECs in environmental media in California and the U.S. West Coast over the period 2012-2022 (Appendix F). The search revealed 25 peer-reviewed articles reporting over 500 substances identified with analytical standards to Level 2 confidence (chemicals with well-defined fragmentation and library spectrum match (Schymanski et al. 2014)). The NTA studies reported only a limited number of compounds with measured water concentrations that were not already in the State Water Board CEC dataset for surface waters. These are included in Appendix E.

The third source of novel chemicals included the UBA database (UBA 2021) and peer-reviewed published papers for studies of CECs in surface waters in California that were not reported in the State Water Board CEC dataset. The database was searched for chemicals reported in studies of surface waters in the USA and Canada. This search yielded MECs for 93 compounds that were not in the State Water Board CEC dataset (Appendix E).

In total 133 compounds were included in the “new CECs” list. A subset of these were assessed as discussed in Chapter 4. Sixteen compounds were selected for prioritization including 6PPD-quinone, a compound highly toxic to coho salmon (*Oncorhynchus kisutch*) and salmonid species (Tian et al. 2021; Brinkmann et al. 2022) (Chapter 6.1.2).

## 3.3 Non-Targeted Analysis (NTA): Instrumental and Bioassay Screening Techniques

Non-target analysis offers a means to identify substances in water that may have not been previously reported. The predominant steps of instrumental NTA of water involve extraction and concentration of substances in water followed by gas chromatography (volatile substances) and liquid chromatography (semi- or non-volatile substances) most commonly coupled to mass spectrometric instrumentation. In addition, *in vitro* bioassays are becoming widely used to screen for types of toxicity relevant to human and/or environmental health and inform the type of CECs that may be present. Thus, effects-directed analyses (EDA) utilize an iterative approach of toxicity screening of water extracts, followed by instrumental NTA. Generally, EDA relies on fractionation of the water extract by polarity, molecular volume, and/or other means.

Over the past 10 years since the original report from this Panel was published, several new developments in both bioanalytical and instrumental NTA have occurred. However, much of the new technologies are related to automation in sample extraction, fractionation, and fluid handling for *in vitro* bioassays. In addition, genomic technology has grown immensely over the past decade and the costs for polymerase chain reaction and sequencing have been reduced. Thus, while reporter gene assays remain the dominant *in vitro* bioassay for water screening, these systems are generally limited to one endpoint (i.e., estrogenicity) and even more limited by the endogenous or synthetic binding site. Regardless, the Panel maintains that bioassays provide additional information of value when screening for new substances in the environment that may have adverse bioactivity. However, as described in detail in the previous report (Anderson et al., 2012), bioassays alone do not identify or quantify any specific chemical or chemicals. Conversely, the bioassay provides a measure of bioactivity related to a specific or general mode of toxicity. If bioactivity is observed in a particular environmental sample, the identification and quantification of the causal substance(s) will require instrumental analytical chemistry approaches. Often, the extract from a particular water sample with bioactivity, as determined using an *in vitro* bioassay, will then be fractionated. In other words, the complex mixture of chemicals within a particular extract will be separated by molecular volume, polarity, volatility, or other means, and collected as individual parcels from the original extract. Fractionation by polarity seems to be the most commonly employed fractionation method. By isolating the bioactivity into a particular fraction(s), the analytical NTA can then be applied to help elucidate the structure(s) responsible for observed toxicity. Ultimately, a mass/activity balance can be evaluated, such that the potency of the particular compounds identified can be added to see if the compounds identified and the quantity present equal the bioactivity observed within the original mixture.

The use of biological assays to monitor water quality is often known as effects-directed analysis (EDA).  According to a survey conducted by the Global Water Research Coalition (GWRC), 75% of water sector stakeholders believed that EDA would improve existing water quality monitoring and over 77% believed that effects-based monitoring would increase consumer confidence about micropollutants in water resources (GWRC

2021). While the majority of respondents indicated that EDA techniques are likely to be more cost effective as compared to targeted monitoring, the limitations for implementation included cost, feedback/support for result interpretation, and lack of guidelines/standards. The GWRC is conducting a comprehensive review of methodologies, trigger values, and decision-making tools for implementation of EDA for water quality and safety assessment (GWRC 2021). Another activity that suggests higher support for *in vitro* assays for water quality and safety assessments comes from the US EPA's decision to eliminate all research and funding for mammalian testing by 2035 (https://www.science.org/content/article/us-epa-eliminate-all-mammal-testing-2035).

One relevant example was published in 2016, which used a glucocorticoid-receptor (GR) reporter gene *in vitro* bioassay with iterative fractionation and high-resolution mass spectrometry, to identify several synthetic glucocorticoid pharmaceuticals which were not previously reported (Jia et al. 2016). Some of the GR compounds discovered and reported for the first time in that manuscript are included in the State Water Board CEC dataset used by the Panel. The authors used an automated solid-phase extraction system to process 1-L water samples. Using high-resolution liquid chromatography with quadrupole time-of-flight (LC-QTOF) technology, several novel GR pharmaceuticals were discovered. After structural identification from LC-QTOF and from review of the literature, a targeted LC-MS/MS method was developed for simultaneous analysis of sub-ng/L concentrations of 26 GR-activating compounds in highly complex natural water matrices (Wu et al. 2019). As compared to the observed bioactivity, four synthetic glucocorticoids (i.e., triamcinolone acetonide, fluocinolone acetonide, clobetasol propionate, and fluticasone propionate) predominantly accounted for the observed GR activity.

In addition to identification of bioactivity, bioassays can also be applied to novel chemicals identified in the environment to provide a general sense of the types and severity of biological effects that may occur through exposure. For instance, a variety of substances have been shown to leach from polymeric-based products, such as tires used predominantly on land transport vehicles. While several recent studies have identified 6PPD quinone as an ichthyotoxic compound in tire leachate (Brinkman et al. 2022), 1,3-diphenylguanidine (DPG) is also commonly used as a secondary accelerator in the sulfur-vulcanization of rubber and other polymers (dos Santos 2022). DPG has been found to be one of the main leachate products of tires and from high density polyethylene pipes and is currently considered ubiquitous in surface waters around the world ranging from low ng/L to mg/L concentrations. Instrumental NTA approaches have been attributed to the detection of DPG in the environment. Fish gastric juices have also been shown to induce DPG leaching from plastics along with a subsequent increase in toxicity (Chen 2021). However, recent research has shown that this ubiquitous environmental contaminant becomes increasingly toxic after chlorination at conditions relevant to drinking water treatment. The increased toxicity includes genotoxicity and altering mitochondrial bioenergetics. Furthermore, using the latest generation of life science tools unveils that several cellular pathways implicated in carcinogenic responses in vivo were activated (i.e., regulation of double strand DNA break repair, DNA recombination, and histone modification). In totality, the future of environmental monitoring will likely depend heavily on NTA techniques that can now be readily combined with the latest generation of genomic and cellular respiration tools.

Since the Panel's previous report, several EDA studies have been undertaken within the State of California. A recently peer-reviewed publication evaluated receptor-based cell bioassays to evaluate estrogen- and glucocorticoid-activity in samples from three California watersheds (Maruya et al. 2022). Similar studies were performed in waters of the Central Valley (Lavado et al. 2009) and San Francisco Bay Delta (Schlenk et al. 2012) as well as the effluent dominated Santa Ana River (Harraka et al. 2021). Most of these studies compared targeted CEC analyses to observed bioactivity. Most samples in the Maruya et al. (2022) study had little to non-detectable bioactivity, with corresponding targeted analyses generally capable of accounting for bioactivity observed. River sediment samples contained certain pesticides (bifenthrin, permethrin, and fipronil) at concentrations that may pose an aquatic risk. In contrast, studies in the Central Valley and San Francisco Bay Delta identified several areas where ER activity was above 100 ng/L of estradiol equivalents. Compounds that co-eluted within active fractions were bifenthrin, diuron, and several nonylphenol compounds (Schlenk et al. 2012). Additional studies in WWTP effluents generally were also positive for estrogen receptor (ER) and GR *in vitro* bioactivity. However, aryl hydrocarbon receptor (AhR) bioactivity was generally not detected or not reported. The Panel discussed the AhR challenges reported by water stakeholders in California, where poor recovery of the positive control (2,3,7,8 TCDD) hindered monitoring efforts. The Panel suggested that a unique sample extraction technique would likely be required for higher TCDD recovery and that the positive controls using polycyclic aromatic hydrocarbons are likely more appropriate to water considering the very low solubility of TCDD. In contrast to water extract studies, evaluations of marine sediment extracts were positive for AhR and GR bioactivity (Crago et al. 2016) and ER activity (Schlenk et al. 2005). Thus, from the data provided to the Panel, the ER and GR bioassays appear to be robust and reliable, whereas the AhR bioassay would require further refinement for sample extraction/preparation/positive controls for application in aquatic ecosystems.

While bioassays offer a wealth of important information regarding the potential for biological effects from discrete CECs and mixtures of substances present in water, regulatory frameworks remain predominantly focused on individual chemicals. For this reason, the identification and quantification of substances remains paramount. Previous panel reports provide in-depth information regarding quality assurance and quality control (QA/QC) measures that are vital to accurate and precise data. Instrumental NTA is particularly difficult to assess the QA/QC as analytical standards are rarely used beyond potential internal standards that may, or may not, be relevant to the compounds identified. Moreover, in general, instrumental NTA is less sensitive as compared to targeted analysis. This can be particularly frustrating when comparing targeted to non-targeted analyses. In multiple studies, NTA was able to identify substances not included in targeted analyses; however, the opposite is also true. Targeted analyses can often quantify compounds that are invisible to NTA due to orders of magnitude greater sensitivity. While NTA is a valuable tool for characterizing complex mixtures of CECs and for compound discovery in environmental matrices when optimally used, it is important to acknowledge such limitations of NTA techniques, as detection and unambiguous identification of unknown compounds remains challenging.

# 4. EFFECTS ASSESSMENT

## 4.1 The Panel's Approach to Identify Monitoring Trigger Levels

The 2022 Panel used an approach similar to that used by the 2012 Panel to determine MTLs for CECs (Anderson et al. 2012). A CEC's MTL is the concentration at which biological endpoints for a species of interest have the potential to be adversely affected, and are derived from the toxicological literature. An important caveat is the discussion below regarding the high level of conservatism inherent to the MTLs presented in this report. With presumably more data available, the Panel anticipated additional certainty regarding the availability of thresholds that could be used to derive MTLs and provide guidance for safety factor assessments. However, toxicity assessments for each of the 300+ chemicals were challenging to identify, mainly because of scarcity of data, and because toxicity studies are rarely performed using similar methods and endpoints by different investigators. The panel reviewed a variety of sources to identify the MTLs, as described below. To err on the side of safety, the panel took the lowest values found in the consulted databases. This conservative approach is likely to be overprotective, but the Panel thought it would be better to use stringent MTLs for chemicals for the application of the risk-based prioritization process, erring on the side of including a CEC that perhaps should not be on list, rather than excluding a CEC that should be on the list. The most important known biological effects for identified CECs were compiled by the Panel and used to assess biological effects of classes of CECs to sentinel species in fresh, estuarine and marine water ecosystems by determining relevant MTLs, in response to Charge Question #5.

The Panel's initial strategy was to use the toxicity levels identified by ASC. However, many toxicity values included in the ASC dataset were defined as 'Predicted No Effect Concentrations (PNECs)', which are concentrations predicted to have no toxicological effect, and are derived using various methods and safety factor assessments. Because the transparency of safety factor assessments was often unclear, instead of relying on the dataset provided by ASC, members of the Panel reviewed toxicity information for each individual chemical on the list of 300+ chemicals of interest, in the various databases described below, identified the most sensitive endpoint, and applied a consistent set of safety factors. The work effort was gargantuan but resulted in a list with uniformly derived conservative MTLs. While most of the data available in databases is for freshwater, the Panel extrapolated values to the other matrices using a uniform set of rules, as described below.

Examples of databases used for threshold determination included values from the U.S. EPA, Office of Pesticide Programs in the form of Aquatic Benchmark values for pesticides https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/aquatic-life-benchmarks-and-ecological-risk#aquatic-benchmarks. Given that Aquatic Benchmark values are not available for other chemicals, MTLs were also obtained from the Computational Toxicology (CompTox) Database https://comptox.epa.gov/dashboard/ and the NORMAN database (https://www.norman-network.com/nds/). Both of these databases have compiled information for thousands of chemicals including pesticides, industrial chemicals, pharmaceuticals, personal care products, and metabolites/degradation products.

Following the identification of a threshold endpoint; Lethal/Effect Concentration affecting 50% (L/EC50; No Observed Effect Concentration (NOEC) or Lowest Effect Concentration (LOEC) were used, various ten-fold (10×) uncertainty factors were applied to threshold endpoint to address uncertainties associated with: extrapolating from acute to chronic endpoints; extrapolating from freshwater to saltwater environments; and whether the compound was listed as an endocrine disruptor on the U.S. EPA CompTox dashboard, or in the literature. Please see Appendix D for examples of how to find MTL information in each of these databases.

The Aquatic Benchmark database was used to determine the MTLs for pesticides (Fig. 4.1). The chemicals are listed in alphabetical order in the database. As shown in the figure, the lowest toxicity threshold value provided by the database for plants, invertebrates, or vertebrate categories was used. For example, the lowest toxicity value identified in the database for atrazine was 1 ug/L for nonvascular plants. In general, thresholds for chronic endpoints tended to be lower than acute endpoints in the Aquatic Benchmark database.

| Pesticide | Year Updated | CAS number | Fish | | Invertebrates | | Nonvascular Plants[5] | Vascular Plants[6] | Office of Water Aquatic Life Criteria | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Acute[1] | Chronic[2] | Acute[3] | Chronic[4] | | | Acute | Chronic |
| Atrazine EXIT | 2016 | 1912-24-9 | 2650 | 5 | 360 | 60 | < 1 | 4.6 | | |

**Figure 4.1. Example screenshot of the U.S. Environmental Protection Agency (EPA) Aquatic Benchmark database output for atrazine, in micrograms per liter (ug/L).**

The CompTox database is the U.S. EPA database that includes a compilation of several databases maintained by EPA in a one-shop format for human and ecological toxicity effects. The database has 906,511 chemicals listed as of August 2022. It is searchable by chemical name or CAS number. Within the CompTox database, the Panel searched chemicals in the Hazard Tab using the point of departure information for Ecological receptors. This is the same information that one would obtain directly from U.S. EPA's Ecotox database. The CompTox database provided endpoints from actual toxicity assays in the form of L/EC 50s, NOECs or LOECs, and identified if the endpoint was reproduction, growth, or survival. The lowest toxicity value available for an aquatic species was selected as the MTL. Toxicity values for terrestrial plants (e.g., lettuce) were not selected for MTL development. If the lowest value available was an acute endpoint, an acute:chronic safety factor was applied (lowest value/10). Exception was given to reproduction studies which were always considered chronic and the acute:chronic safety factor was not applied.

The Panel prioritized values for reproduction over those for growth or survival or for any biochemical or histological response. The rationale for the focus on reproduction was that for most compounds, reproduction was a chronic endpoint that is more closely aligned with population impacts. However, in some instances reproduction was listed as an "acute" response based upon the duration of exposure rather than the effect. In those cases, "acute" response thresholds were lower than "chronic" response thresholds. If survival was used as an endpoint, then the $50^{th}$ percentile was used. If reproduction was used, then the NOEC or LOEC was used. If the LOEC was lower than the NOEC, then the LOEC was used.

In addition to toxicity information, the Panel determined if a chemical was an endocrine disruptor by looking at the Executive Summary page for each chemical where U.S. EPA assigns chemicals as to their potential for endocrine activity, based mainly on their bioactivity assays with estrogen and androgen receptors. The Panel used the information as presented by U.S. EPA. Information for how the Panel navigated this database is shown in Appendix D. However, in some cases (e.g., atrazine), the literature was used to determine whether a compound should be categorized as an EDC. It is likely that future expert analyses may be needed to confirm identification.

The NORMAN database is a network of information maintained in Europe but also including many countries around the world that also houses a collection of databases for information on chemicals in the environment. The NORMAN "Ecotoxicology Database" lists values for over 94,418 chemicals based on either experimental endpoints from ecotoxicology assays or predicted by quantitative structure-activity (QSAR) models. The experimental studies are available in a range of matrices including freshwater, marine water, sediments, and tissue. They include values from acute and chronic studies. Only 2,197 chemicals, however, have PNECs derived experimentally, so the vast majority come from QSAR models based on *Selenastrum capricornutum*, *Daphnia magna*, or fathead minnow (*Pimephales promelas*). In most cases, the NORMAN database applied a series of safety factors that ranged from 10 to 1,000. The QSAR-based values were predicted as 72 hr $EC_{50}$values for *Selenastrum capricornutum*, 48 h $LC_{50}$ values for *Daphnia magna,* or 96 h $LC_{50}$ values modeled for fathead minnow. In those cases, safety factors were removed and final MTLs were derived using the Panel's recommended safety factor assessment strategy. Lastly, literature-based thresholds using the endpoints above were also used in some cases with subsequent application of safety factors depending upon the uncertainty of the matrix or the endpoints (see below).

As shown in Figure 4.2, once the occurrence dataset was vetted for quality assurance and control, toxicity values were evaluated from the databases above or the scientific literature. In general, preference was given to U.S. EPA Aquatic Benchmarks (Pesticides) and CompTox data with subsequent use of the NORMAN database, if the compound was not found in CompTox.

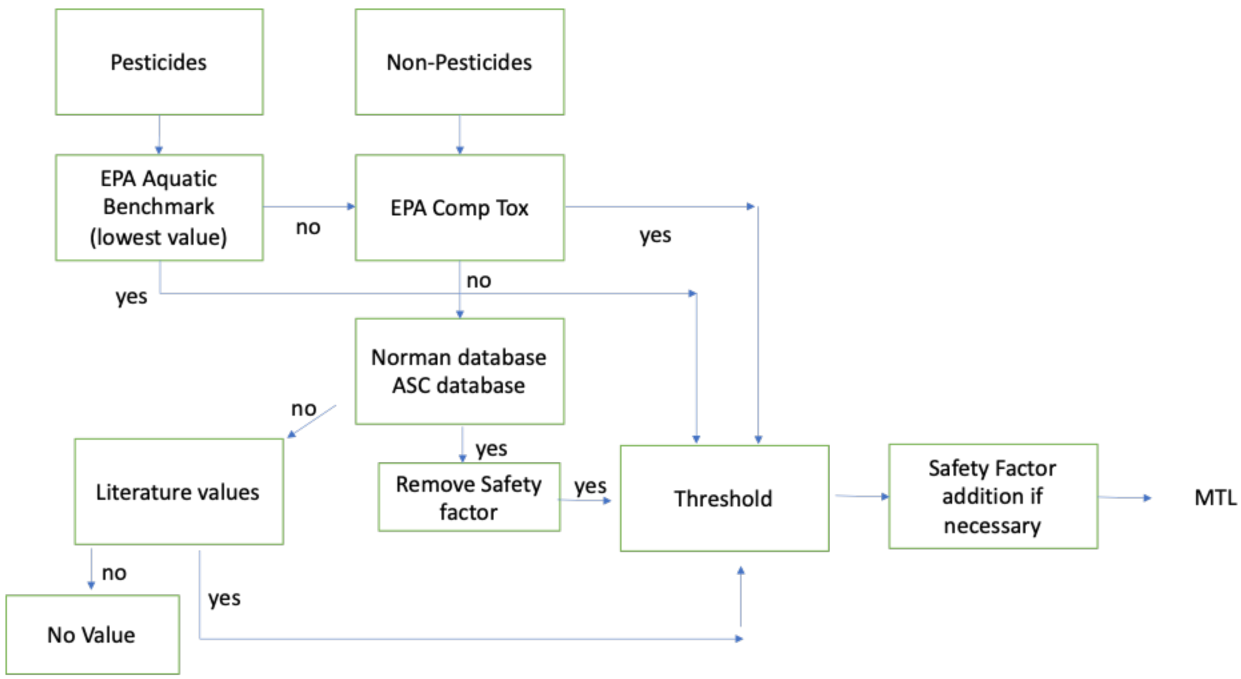


**Figure 4.2. Conceptual framework to derive monitoring trigger levels (MTLs).**

For the selection of toxicity endpoints, species sensitivity distribution values (i.e., effect concentrations of the 5th or 10th percentiles) were preferred over reproduction NOECs. If reproduction NOECs were not available, impaired growth, or survival NOECs were used. If NOECs were not available or if they did not provide the lowest threshold, LOECs were utilized. If chronic or reproduction endpoints were not available, then acute values of toxicity (i.e., $LC_{50}$-lethality or $EC_{50}$-growth) were used and a 10-fold uncertainty factor was applied to the acute value to account for the uncertainty associated with the acute to chronic extrapolation. 10-fold safety factors were also applied if the EPA Comp Tox database indicated a significant endocrine disruption identification, or the literature showed significant endocrine effects for the compound (Figure 4.3).

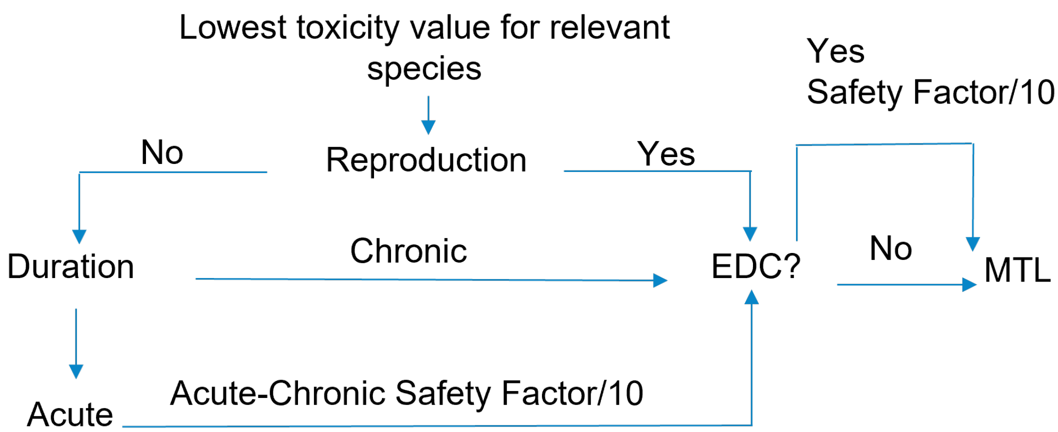


**Figure 4.3. Flow chart of calculations for monitoring trigger levels (MTls) from database endpoint selections.**

When deriving marine or estuarine water MTLs based on a freshwater MTL, a 10-fold uncertainty factor was applied. While recent studies of 104 different organic and inorganic compounds have indicated no significant differences in acute toxicity between freshwater and saltwater (Yanaigihara et al. 2022), other studies have shown significant increases in toxicity in saltwater compared to freshwater. The increase in toxicity may be structurally mediated and focused on sublethal toxic responses (Schlenk and Lavado 2011). Consequently, with the goal of including rather than excluding a CEC in the monitoring program, the Panel selected a more conservative approach by applying a 10-fold freshwater to saltwater uncertainty factor. However, it is recommended that endpoints from marine species from CompTox, NORMAN or peer-reviewed literature be utilized to derive MTLs for that matrix. For the MTLs calculated in this report, only freshwater organism MTLs were used with subsequent safety factor adjustments to determine saltwater MTLs. There are a few chemicals for which saltwater values exist in these databases. These were not used in this report.

While MTLs for the sediment matrix are not the focus of this report, the Panel provided training to State Water Board staff in how to develop these values. MTLs for the sediment matrix would be derived using an approach similar to that used for the freshwater matrix. Essentially, NOECs would be targeted with the lowest value prioritized, and if not available, a 10-fold uncertainty factor would be applied to account for uncertainties associated with the acute to chronic extrapolation. (Note that in this report, the term “uncertainty factor” is used interchangeably with “safety factor”.) A 10-fold uncertainty factor for EDC potential would be used if the compound was identified as such by the U.S. EPA CompTox database, and a 10-fold uncertainty factor would be applied to derive estuarine/marine sediment MTLs if toxicity values were unavailable for organisms in this medium.

## 4.2 Other Approaches to Derive MTLs

In cases where no MTLs for CECs can be adopted from established toxicity databases as described in Chapter 4.1, there are only a few methods to perform read across among species. One excellent method is the use of the web-based program entitled Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS; https://seqapass.epa.gov/seqapass/). This program predicts how a chemical may act across species by quantifying the *in silico* determined binding affinity of chemicals for their receptors in the species depending on the similarity of amino acids within a binding pocket. This approach is useful when moving to "*in silico*" approaches when expanding risk assessment to sensitive species.

In the future, based on the concept of Adverse Outcome Pathways, it may be possible to determine the likely initiating molecular event (MIE) that leads to adversity in apical endpoints that are useful for risk assessment. These initiating molecular events can be measured by *in vitro* assays using cells rather than whole organism toxicity tests. Currently AOPs are qualitative, but the field is moving to determining quantitative AOPs. The U.S. EPA is developing high throughput assays that can be used in this manner and validating them through *in vitro* to *in vivo* experiments that show that the initiating molecular event is essential through key events to result in adversity at the apical level. They have developed over 700 assays to cover over 300 signaling pathways (https://www.epa.gov/chemical-research/toxcast-data-generation-toxcast-assays). This database will be useful in the future to develop MTLs as *in vitro* to *in vivo* experiments are validated to compare $EC_{50}$ values. While these methods are still in their infancy, there is likely considerable movement within the U.S. EPA to use this type of assay in the future.

# 5. Overview of the Process to Identify and Prioritize CECs for Monitoring and Further Evaluation

This chapter and Chapter 6 describe the process recommended by the Panel to identify CECs to be included in a monitoring program or that may require further evaluation other than monitoring in response to Charge Questions # 2 and 6. The general approach follows the risk-based screening process recommended by the 2012 Panel's earlier report (Anderson et al. 2012). Namely, derivation of a monitoring trigger quotient (MTQ) by dividing either the CEC-specific MEC or predicted environmental concentration (PEC) by the CEC-specific MTL. Given the existence of a substantially larger California-specific dataset than what was available in 2012, the screening process has been updated to prioritize CECs for monitoring based on a combination of the magnitude of the MTQ, and the presence or absence of a trend in concentration, sample size and differences between $MTQ_{detect}$ than $MTQ_{sub}$ considering the State Water Board dataset. The CEC identification and monitoring prioritization process is not uniquely applicable to the State Water Board dataset. If other datasets have available monitoring data, the prioritization process can be applied to those as well. However, in this report, the process is applied to just the State Water Board dataset and additional data sources.

The overall CEC identification and prioritization process is divided into two screening stages as illustrated in Figure 5.1. The first stage consists of a conservative preliminary monitoring prioritization screening described in Chapters 5.1 and 5.2. The second stage is a refined monitoring prioritization (described in Chapter 6.2) that takes into account considerations such as sample size, differences between $MTQ_{detect}$ and $MTQ_{sub}$,, geographic and temporal distribution of monitoring data to evaluate the presence of trend, and comparison of method detection limits to MTLs.

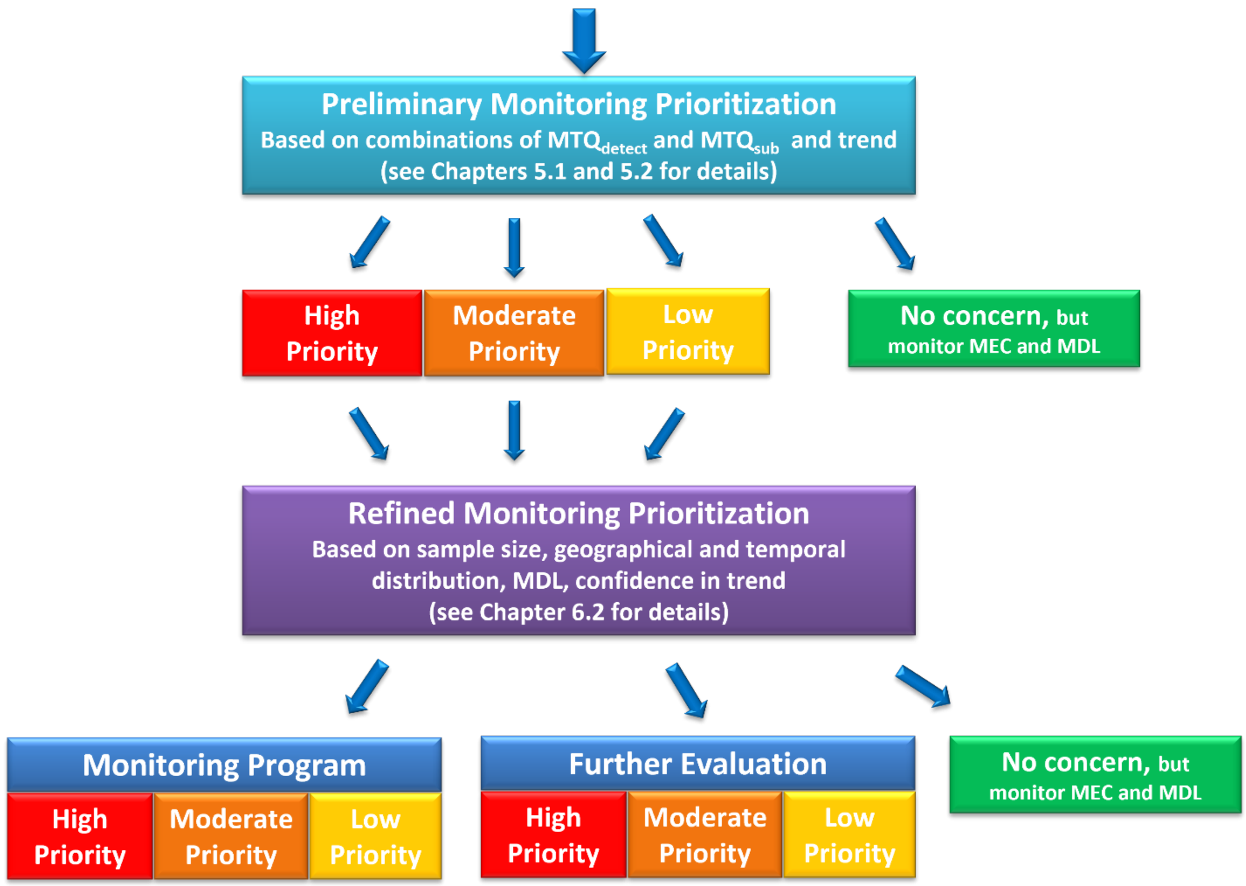


**Figure 5.1 Overview of the process to identify and prioritized constituents of emerging concern (CECs) for monitoring and further evaluation.**

## 5.1 Overview of Preliminary Monitoring Prioritization

Before describing the updated risk-based monitoring prioritization process, the Panel wishes to emphasize that the MTQs generated as part of the prioritization process described below (in this Chapter and Chapter 6) cannot and should not be interpreted as representing estimates of potential risk. As was the case with the CEC screening process developed in 2012, categorizing a CEC as a monitoring priority based on its MTQ does not mean the CEC poses a potential risk, but rather only that the CEC warrants further investigation. Several conservative assumptions were used to establish the MEC and the MTL. Based on those conservative assumptions, the State can be confident that MTQs of less than one (1) indicate a CEC is not a monitoring priority and that MTQs of greater than 1 indicate the need for review of the assumptions used to derive the MTL and MEC to confirm they are representative. It is only after such review that an appropriate MTQ can be derived, and the monitoring priority of a CEC established.

The key reason for updating the CEC screening process presented in the 2012 report (Anderson et al. 2012) is the existence of a decade or more of California-specific monitoring data for CECs. Those data can be parsed into specific time periods and evaluated for trends in occurrence concentrations. The Panel views information about trend as a window into how concentrations of a CEC may change in the future providing an "early warning system" of sorts. For example, if a CEC has an MTQ < 1 based on the most recently collected data but the MTQ is trending upwards, that may be an indication the MTQ may exceed 1 in the future. As a result, that CEC may warrant higher monitoring priority than its current MTQ would suggest. While the Panel views trend information as important, the Panel also wishes to emphasize and caution that currently available data in the State Water Board dataset are insufficient for statistically rigorous trend analysis. The evaluation of trend applied in this report is based simply on the ratio of the most recent to the next most recent $MEC_{detect}$ (i.e., $MEC_{detect,2021} \div MEC_{detect,2015}$ or $MEC_{detect,2015} \div MEC_{detect,2010}$) or $MEC_{sub}$ (i.e, $MEC_{sub,2021} \div MEC_{sub,2015}$ or $MEC_{sub,2015} \div MEC_{sub,2010}$).

Four categories of trend are defined in the identification and prioritization process:

- a ratio of >2.5 is assumed to represent a steeply increasing trend;
- a ratio of >1.5 and ≤2.5 is assumed to represent a gradually increasing trend;
- a ratio of ≥0.7 and ≤1.5 is assumed to represent the absence of a trend; and
- a ratio <0.7 is assumed to represent a decreasing trend.

If in the future the availability of monitoring data allows, the Panel encourages use of methods that will result in a more rigorous evaluation of trend.

## 5.2 Screening logic to identify relevant CECs for monitoring including MTQs

To conduct the preliminary monitoring prioritization, available data and MTLs are used to calculate an $MTQ_{detect}$, $MTQ_{sub}$ and trend. If data are available, MTQs and trend can be calculated for all environmental media (e.g., fresh, marine water, estuarine water, sediment and tissue). Additionally, when data are available, MTQs and trend can be calculated for each matrix within an environmental medium (for example, for total and dissolved concentrations of samples from fresh, estuarine, or marine waters).

The preliminary monitoring prioritization process categorizes CECs as either needing to be retained for possible inclusion in a monitoring program or eliminated from consideration in a current monitoring program. CECs that are eliminated from consideration in a monitoring program based on current data can be evaluated again using the preliminary monitoring prioritization screening process if additional data are collected or if MTLs change. CECs that are retained for possible inclusion in a monitoring program are categorized as having either ‘High’, ‘Moderate’ or ‘Low’ monitoring priority (Figure 5.2).

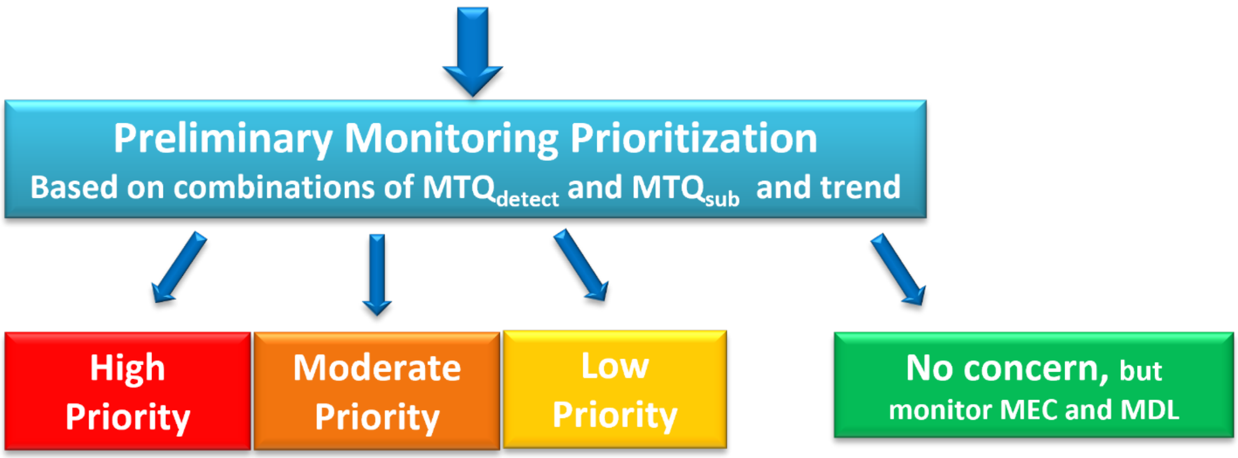


**Figure 5.2. Overview of the preliminary monitoring prioritization.**

Within each prioritization category, CECs are further divided depending upon the specific combination of MTQ and change in temporal concentration, if available (e.g., A1, A2, or A3 in the ‘High’ priority category; Figure 5.3). The point of the various levels within each monitoring priority category was to better understand what aspect of the monitoring prioritization framework (e.g., magnitude of MTQ, temporal change in concentration, detected vs substituted MECs) was causing a particular categorization. That information, in turn, can be used to focus subsequent evaluations needed to refine the initial monitoring prioritization.

Change in temporal concentration is an additional line of evidence. As an example, consider two compounds with 0.1<MTQ<1. In a strictly MTQ-based monitoring prioritization framework, such compounds would not be included on a monitoring list. However, if available information indicates the concentration of one of those compounds is increasing over time, it would be a candidate for monitoring to understand whether concentrations are going to continue to increase in the future and MTQs exceed unity. That is why compounds with MTQ<1 can still be categorized as “High”, “Moderate” or “Low” monitoring priority (see monitoring priority bases A3, B2, B3, C3 in Figure 5.3) and as described below.

| $MTQ_{detect}$ | ≥10 | 1-10 | 1-10 | 1-10 | >10 |
|---|---|---|---|---|---|
| Condition | or | or | or | or | or |
| $MTQ_{sub}$ | ≥10 | 1-10 | 1-10 | 1-10 | >10 |
| Trend | | ↑↑ | ↑ | = or ↓ | ID |
| Monitoring Priority | High | High | Mod | Low | Low |
| Monitoring Priority Basis | A1 | A2 | B1 | C1 | C2 |

| $MTQ_{detect}$ | 0.1-1 | ≤0.1 | 0.1-1 | ≤0.1 | ≤1 | ≤0.1 | 0.1-1 |
|---|---|---|---|---|---|---|---|
| Condition | or | and | or | and | and | and | Or |
| $MTQ_{sub}$ | 0.1-1 | ≤0.1 | 0.1-1 | ≤0.1 | ≤1 | ≤0.1 | 0.1-1 |
| Trend | ↑↑ | ↑↑ | ↑ | ↑ | = or ↓ | ID | ID |
| Monitoring Priority | High | Mod | Mod | Low | Out | Out | Low |
| Monitoring Priority Basis | A3 | B2 | B3 | C3 | D1 | D2 | C4 |

Trend key

↑↑: Steeply increasing trend ($MEC_{detect}$ or $MEC_{sub}$ ratio >2.5 between most recent two time periods).

↑: Gradually increasing trend ($MEC_{detect}$ or $MEC_{sub}$ ratio >1.5 and <2.5 between most recent two time periods).

=: Stable trend ($MEC_{detect}$ or $MEC_{sub}$ ratio >0.7 and <2.5 between most recent two time periods).

↓: Decreasing trend ($MEC_{detect}$ or $MEC_{sub}$ ratio <0.7 between most recent two time periods).

ID: Insufficient data to calculate trend.

**Figure 5.3. Preliminary Monitoring Prioritization Categories, based on values for Monitoring Trigger Levels for both detected data ($MTL_{detect}$) and substituted data ($MTL_{sub}$), temporal trends over time for Measured Environmental Concentrations for detected data ($MEC_{det}$) and substituted data ($MEC_{sub}$), and the potential for insufficient trend data (ID).**

CECs are categorized as having a 'High' monitoring priority under three conditions:

- $MTQ_{detect}$ or $MTQ_{sub}$ ≥10, regardless of trend (Monitoring Priority Basis A1);
- 10 > $MTQ_{detect}$ or $MTQ_{sub}$ >1 and a steeply increasing MEC trend (Monitoring Priority Basis A2); and
- 1≥ $MTQ_{detect}$ or $MTQ_{sub}$ ≥0.1 and a steeply increasing MEC trend (Monitoring Priority Basis A3).

CECs are categorized as having a 'Moderate' monitoring priority under three conditions:

- 10 > $MTQ_{detect}$ or $MTQ_{sub}$ >1, and a gradually increasing MEC trend (Monitoring Priority Basis B1);
- 1≥$MTQ_{detect}$ and $MTQ_{sub}$ ≥0.1 and a steeply increasing MEC trend (Monitoring Priority Basis B2); and

- $1 \geq MTQ_{detect}$ or $MTQ_{sub} \geq 0.1$ and a gradually increasing MEC trend (Monitoring Priority Basis B3).

CECs are categorized as having a ‘Low’ monitoring priority under four conditions:

- $10 > MTQ_{detect}$ or $MTQ_{sub} > 1$, and either no MEC trend or a decreasing MEC trend (Monitoring Priority Basis C1);
- $10 > MTQ_{detect}$ or $MTQ_{sub} > 1$, and insufficient data to determine a MEC trend (Monitoring Priority Basis C2);
- $MTQ_{detect}$ and $MTQ_{sub} \geq 0.1$ and a gradually increasing MEC trend (Monitoring Priority Basis C3); and
- $1 \geq MTQ_{detect}$ or $MTQ_{sub} \geq 0.1$ and insufficient data to determine a MEC trend (Monitoring Priority Basis C4).

CECs are eliminated from consideration in the current monitoring program under two conditions:

- $MTQ_{detect}$ and $MTQ_{sub} \leq 1$ , and either no MEC trend or a decreasing MEC trend (Monitoring Priority Basis D1); and
- $MTQ_{detect}$ and $MTQ_{sub} \leq 0.1$, and insufficient data to determine a MEC trend (Monitoring Priority Basis D2).

As was the case with the CEC screening process developed in 2012, categorizing a CEC as ‘High’ monitoring priority does not mean the CEC poses a potential risk. Several conservative assumptions were used to establish the MEC (or PEC) and the MTL. The Panel felt use of such conservative assumptions was appropriate for determining whether a CEC should be included in a monitoring program. Such conservative assumptions need to be refined prior to determining whether a potential risk may actually be present. Moreover, just because a CEC is categorized as a ‘High’ monitoring priority following the preliminary monitoring prioritization process, additional refinement of the assumptions used in the preliminary prioritization may lead to a change in monitoring priority. Such additional refinements can include consideration of sample size, geographic and temporal distribution of available monitoring data, and comparison of method detection limits to MTLs (Figure 5.4). For example, if an MTQ > 1 or an increasing trend is based on elevated or increasing method detection limits, further evaluation of analytical methods for that CEC as opposed to inclusion of that CEC in a monitoring program may be the next step. Additional evaluations of the MTL choice may also be warranted as uncertainties exist often in the use of nominal exposure concentrations for bioassay-derived thresholds which may not be accurate. In some cases, the effect threshold may be lower than the analytical method for detection in the environment or the assay system itself. Such potential refinements are described in more detail in Chapter 6.2.

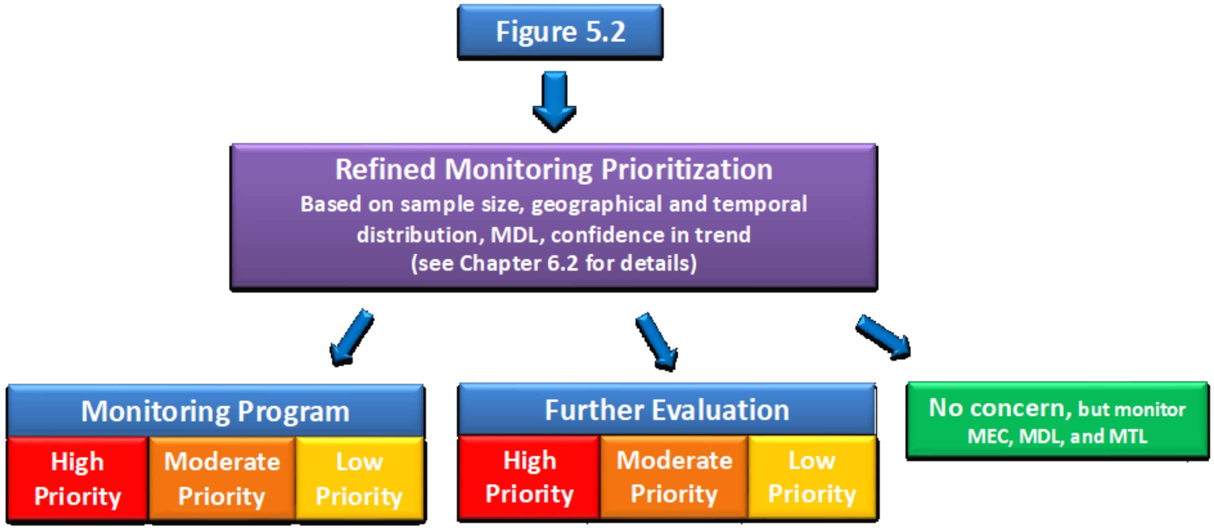


**Figure 5.4. Refined monitoring prioritization to identify relevant constituents of emerging concern (CECs) for monitoring.**

# 6. APPLYING THE RISK-BASED SCREENING FRAMEWORK TO IDENTIFY RELEVANT CECS FOR AMBIENT WATERS

Chapter 6.1 presents the results of the application of the preliminary monitoring prioritization framework (Chapter 5) to the current fresh, estuarine and marine water State Water Board dataset to identify CECs and classes of CECs that have the potential to adversely impact marine, estuarine and freshwater wildlife, ecosystems, and beneficial uses in marine, estuarine and freshwater environments (in response to Charge Question #1). Chapter 6.2 describes a refined monitoring prioritization framework (in response to Charge Question #2) and its application to eight example CECs. Chapter 6.3 summarizes persistence and bioaccumulation information about CECs evaluated in this report and how those could be accounted for in a monitoring prioritization program. Chapter 6.4 discusses aspects of the design of monitoring and evaluation programs for CECs depending upon a refined monitoring priority to provide the State Water Board with a transparent and informed prioritization framework for the most relevant CECs (in response to Charge Question #6).

## 6.1 Identification of Possible CECs in Different Matrices Based on Measured Environmental Concentrations and Trends

The decision framework documented in Chapter 5 has been embedded in the State Water Board CEC Dashboard for fresh, estuarine and marine water sample matrices as well as sediments and tissues. Applying this preliminary monitoring prioritization framework to the occurrence data (Appendix H, Tables H.1 to H.3) within the State Water Board CEC dataset results in preliminary short-lists of CECs (Appendix I, Tables I.1 to I.12) with different monitoring priorities (i.e., 'High' – 'Moderate' – 'Low' – 'Out' (not a priority)) for each matrix. The outcome of applying the preliminary monitoring prioritization framework to the occurrence data in California for fresh, estuarine, and marine waters is described in Chapter 6.1.1. The same logic can be applied to other environmental matrices including sediments and tissues.

### 6.1.1 Prioritizing a preliminary monitoring shortlist of CECs in freshwater using the State Water Board CEC Dashboard

Following application of the preliminary monitoring prioritization framework to the current State Water Board freshwater dataset, 105 CECs were classified as 'High' priority (Appendix I, Table I.1), 30 CECs were classified as 'Moderate' priority (Appendix I, Table I.2), 56 CECs were classified as 'Low' priority (Appendix I, Table I.3), and 103 CECs were classified as not a monitoring priority (Appendix I, Table I.4). As noted previously, the preliminary monitoring prioritization framework is intended to be conservative. In other words, to err on including CECs in the monitoring program rather than inadvertently exclude a CEC that should have been included. The refined monitoring prioritization framework presented in Chapter 6.2 delves deeper into the available information about occurrence (e.g., frequency of detection, temporal and geographical spread, MDL) to update the results of the preliminary monitoring prioritization framework.

For comparison, Table 6.1 summarizes the CECs with a risk quotient MTQ larger than 1 for freshwater matrices proposed by the previous 2012 Panel.

**Table 6.1 Constituents of emerging concern (CECs) with monitoring trigger quotients (MTQs) greater than unity (>1) for aqueous exposures in inland waterways proposed by the 2012 Panel. Units are in nanograms per liter (ng/L) for the measured environmental concentration (MEC), no observed environmental concentration (NOEC), predicted no effects concentration (PNEC), and monitoring trigger levels (MTL). [a]Endocrine disrupting compound (EDC) mode of action not incorporated into PNEC or NOEC. [b]Unknown mode of action.**

| Compound | MEC (ng/L) | Toxicity Thresholds (NOEC or PNEC) (ng/L) | Safety Factor | Freshwater MTL (ng/L) | MTQ |
|---|---|---|---|---|---|
| Bifenthrin | 85 | 4 | 10 [a] | 0.4 | 210 |
| Permethrin | 46 | 10 | 10 [a] | 1 | 46 |
| Chlorpyrifos | 190 | 50 | 10 [a] | 5 | 38 |
| Estrone | 73 | 6 | 1 | 6 | 12 |
| Ibuprofen | 1000 | 1000 | 10 [b] | 100 | 10 |
| Bisphenol A | 520 | 60 | 1 | 60 | 8.7 |
| 17-beta estradiol | 8.4 | 2 | 1 | 2 | 4.2 |
| Galaxolide (HHCB) | 2780 | 7000 | 10 [b] | 700 | 4.0 |
| Diclofenac | 230 | 1000 | 10 [b] | 100 | 2.3 |

### 6.1.2 Prioritizing a preliminary monitoring shortlist of CECs in freshwater using the additional MEC sources

To conduct a comprehensive review of new CECs, the Panel reviewed other sources including the UBA database (UBA. 2021), and from peer-reviewed published papers for studies of CECs in surface waters in California that were not reported in the State Water Board CEC dataset. Several of the studies used NTA to identify CECs in surface waters in California and the U.S. West Coast. The UBA database was searched for measured values of pharmaceuticals in surface waters of the USA and Canada only. Because these sources are new and the measured data are limited, the Panel was not able to determine 90$^{th}$ percentiles. However, the Panel did identify toxicity values for some of the chemicals in this list. The comprehensive list of 133 chemicals, including their measured concentrations and MTLs are found in Appendix E. The Panel was unable to derive MTLs for 23 of these substances including several estrogen metabolites, among others. For the chemicals for which MTLs could be derived, tentative MTQs were calculated. Most of the measured concentrations for this list of substances were much lower than the MTLs, placing them into the No Concern category. However, based upon MTQ measurements, 21 compounds were identified in freshwater matrices that had MTQs above unity. The MTQs ranged from low single digits to over 1,000,000 (Appendix E). Consideration of these chemicals for possible inclusion in a CEC monitoring list is warranted to understand their concentrations and geographic extent in

California surface waters better. Two examples include the veterinary pharmaceutical agent ivermectin and the tire-derived antioxidant additive chemical *N*-(1,3-Dimethylbutyl'-*N*'-phenyl-p-phenylenediamine-quinone (6PPD-quinone).

### *Ivermectin*

The maximum MEC for ivermectin was 0.088 ug/L and the MTL determined from empirical data in CompTox was $3 \times 10^{-7}$ ug/L. An alternative MTL derived from the NORMAN database as a predicted QSAR was 0.142 ug/L. Since CompTox was prioritized as a primary database, the MTQ was 293,000. To confirm this value, other endpoints for the MTL were searched using CompTox and found to be consistent. The value for the MEC was identified from the literature with subsequent evaluations of the QA/QC and confirmed to be appropriate. No monitoring data from California were reported in the State Water Board dataset or found in the literature. Given the high MTQ, this would be an example of a compound of ‘High’ priority informed by sources other than the State Water Board dataset.

### *6PPD-quinone*

The mean MEC of 6PPD-quinone was 1.9 ug/L and the maximum MEC was 3.5 ug/L. While listed in CompTox with 30 ug/L in zebrafish, a more recent publication (Brinkmann et al., 2022) indicated the MTL in salmonid fish species was 0.059 ug/L resulting in MTQs of 32.2 and 59.3, respectively. Occurrence data has been observed in California and confirmed as high quality.

## 6.1.3 Prioritizing a preliminary monitoring shortlist of CECs in Estuarine water bodies using the State Water Board CEC Dashboard

Following application of the preliminary monitoring prioritization framework to the current State Water Board marine dataset, 51 CECs were classified as ‘High’ priority for estuarine water bodies (Appendix I, Table I.5), 17 CECs were classified as ‘Moderate’ priority (Appendix I, Table I.6), 48 CECs were classified as ‘Low’ priority (Appendix I, Table I.7), and 161 CECs were classified as not a monitoring priority (Appendix I, Table I.8). Again, the preliminary monitoring prioritization framework is intended to be conservative and err on including CECs in the monitoring program rather than inadvertently exclude a CEC that should have been included. Refined monitoring prioritization is presented in Chapter 6.2.

### 6.1.4 Prioritizing a preliminary monitoring shortlist of CECs in marine water bodies using the State Water Board CEC Dashboard

In a manner analogous to that of Chapters 6.1.2 and 6.1.3, 26 CECs were classified as 'High' priority (Appendix I, Table I.9), no CECs were classified as 'Moderate' priority, 19 CECs were classified as 'Low' priority (Appendix I, Table I.11), and 30 CECs were classified as not a monitoring priority (Appendix I, Table I.12). As noted previously, the preliminary monitoring prioritization framework is intended to be conservative and err on including CECs in the monitoring program rather than inadvertently exclude a CEC that should have been included. The refined monitoring prioritization framework presented in Chapter 6.2 delves deeper into the available information about occurrence to update the results of the preliminary monitoring prioritization framework.

### 6.1.5 Effect of using median MDL on MTQs

The $MTQ_{sub}$ was used for 224 of the 339 CECs of the preliminary prioritization (Appendix I, Table I.12). Thus, it was of interest to see the effect of substitution of the median detection limit by calculating the ratio of the 90$^{th}$ percentile concentrations with substitution ($MEC_{sub}$) divided by 90$^{th}$ percentile concentrations without substitution ($MEC_{detect}$) (Appendix I.12). Because the median MDLs were higher than some measured concentrations for about 135 of the 339 CECs, the ratios were >1. However, the substitution made <10-fold difference for 122 of 236 CECs for which ratios could be calculated. In fact, the measured $MTQ_{detect}$ was used for 79 of the 122 CECs. The largest ratios (>100, highlighted as category "A" in Table I.12) were for 71 of the 236 CECs. These were CECs having relatively few detected concentrations along with reported detection limits that were higher than measured concentrations in some cases. A subset of the 339 CECs did not have ratios calculated due to lack of measured data to estimate 90$^{th}$ percentiles. This topic is further discussed in Chapter 2.1.1 in connection with the range of MDLs reported by various monitoring programs contributing to the State Water Board dataset.

## 6.2 Refining Monitoring Prioritization for CECs

As described in Chapter 5, the preliminary monitoring prioritization framework uses several assumptions that are intentionally conservative and is designed to err on the side of including CECs for consideration in a monitoring program rather than excluding them. As shown in Chapter 6.1, this can result in identifying a large number of CECs for potential inclusion in a monitoring program. Not all such CECs may warrant inclusion if some of the conservative assumptions used in the preliminary monitoring prioritization framework are found to be too conservative or not supported following further examination of the data. Chapter 6.2.1 presents a refined monitoring prioritization framework and Chapter 6.2.2 applies the refined framework to five example CECs identified as having either a high or moderate monitoring priority based on the preliminary monitoring prioritization framework and the freshwater State Water Board dataset, as well as two example CECs identified as having a high monitoring priority based on the marine State Water Board dataset, and one example CEC identified as having high priority based on the estuarine dataset (Chapter 6.1).

### 6.2.1 Description of the refined monitoring prioritization decision framework

The refined monitoring prioritization framework consists of criteria specified in an MTQ selection Table (Table 6.2.1) and 10 decision tree diagrams (Appendix G, Figures G.1 through G.10). The MTQ selection table is used to determine whether the $MTQ_{detect}$ or $MTQ_{sub}$ will be used in the monitoring refinement prioritization. Each of the decision diagrams corresponds to one of the 10 preliminary monitoring prioritization outcomes shown in Figure 5.3. The MTQ selection table was necessary to address the uncertainty regarding MDLs in the current State Water Board dataset.

Given the uncertainty surrounding MDLs, in almost all cases where both the $MTQ_{sub}$ and $MTQ_{detect}$ are available and can be compared relative to the threshold of 1, refined prioritization is based on the $MTQ_{detect}$. Preference is given to the $MTQ_{detect}$ because detected concentrations better represent ambient concentrations in surface water than $MTQ_{sub}$, given the uncertainty surrounding MTLs in the current State Water Board dataset. The $MTQ_{sub}$ includes non-detected concentrations that may be elevated because of variability of analytical methods used to date. The one exception to the general rule is when $MTQ_{detect}$ >1 but $MTQ_{sub}$ ≤1. In that case, $MTQ_{sub}$ is used for refined prioritization as it likely represents a distribution of concentrations dominated by non-detects with reasonable detection limits and a smaller number of samples with detected concentrations.

**Table 6.2.1 Selection of monitoring trigger levels (MTQs), either for substituted values ($MTQ_{sub}$) or detected values ($MTQ_{detect}$) to use in the refined prioritization decision tree diagrams of Appendix G (Figures G.1 to G.10).**

| $MTQ_{detect}$ | $MTQ_{sub}$ |
|---|---|
| >1 (selected) | >1 |

| | |
|---|---|
| >1 (selected) | ≤1 |
| ≤1 | >1 (selected) |
| ≤1 (selected) | ≤1 |

## 6.2.2 Application of the refined monitoring prioritization framework to five example freshwater, two example marine water, and one example estuarine water CECs

Application of the refined monitoring prioritization framework consists of first applying the MTQ selection table (Table 6.2.1) to determine which MTQ will be used in the refinement. Once either $MTQ_{detect}$ or $MTQ_{sub}$ is selected, the decision tree diagram corresponding to a CEC's preliminary monitoring prioritization category is used to refine the prioritization. In addition, refinement may be required for the MTL as discussed above where more accurate thresholds may be identified from the literature or from other studies in the database that have appropriate QA/QC (i.e., measured chemistry of exposure). Application of the refinement process is presented below for five example freshwater CECs and three example marine CECs, all with a 'High' preliminary monitoring prioritization category.

### *6.2.2.1 Azithromycin*

The refined monitoring prioritization is based on concentrations reported for the dissolved freshwater matrix. No concentrations are available for the total freshwater matrix.

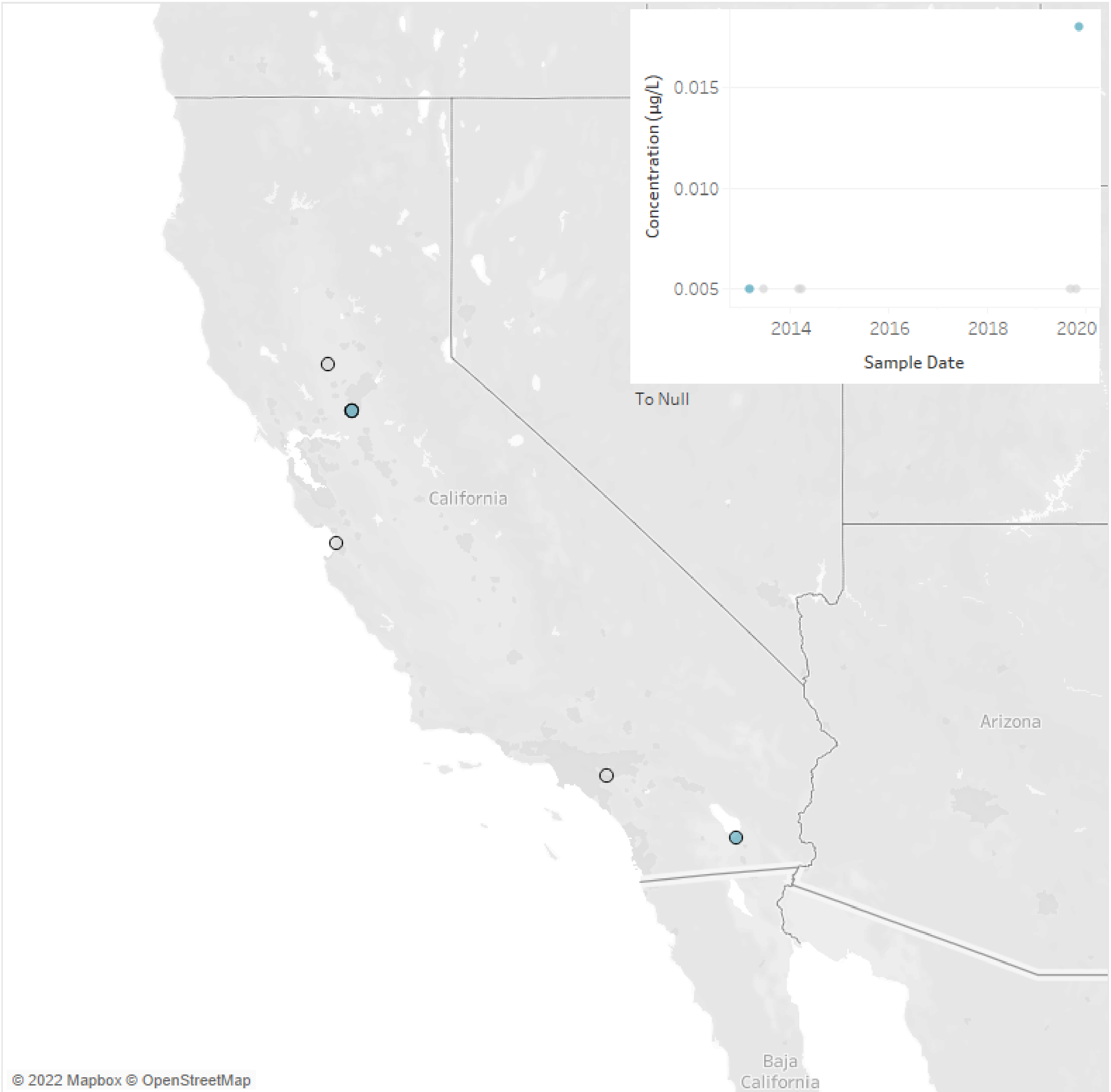


**Figure 6.1. Azithromycin in freshwater, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

Preliminary monitoring prioritization outcome

- $MTQ_{detect}$ <1 (0.001); trend >2.5 (3.6), N<10 (2)
- $MTQ_{sub}$ <1 (0.0006), trend >2.5 (3.6), N<10 (7)
- Preliminary Monitoring Prioritization: **B2**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1.)
    - Both $MTQ_{detect}$ and $MTQ_{sub}$ available and ≤1. Monitoring refinement based on $MTQ_{detect}$.
- B2 Refined Decision Framework Figure
    - Outcome based on current refined decision framework:
        - $MTQ_{detect}$ >0.1 and ≤1, N<10; Special Study: Evaluate need for additional monitoring.

Based on the refined monitoring prioritization, the preliminary monitoring prioritization of Moderate (B2) for azithromycin changes to needing additional evaluation (Special Study) to determine whether monitoring is required given that the $MTQ_{detect}$ is between 0.1 and 1 and the sample size is less than 10.

### *6.2.2.2 Di-2-ethylhexyl phthalate*

The refined monitoring prioritization is based on concentrations reported for the total freshwater matrix. No concentrations are available for the dissolved freshwater matrix.

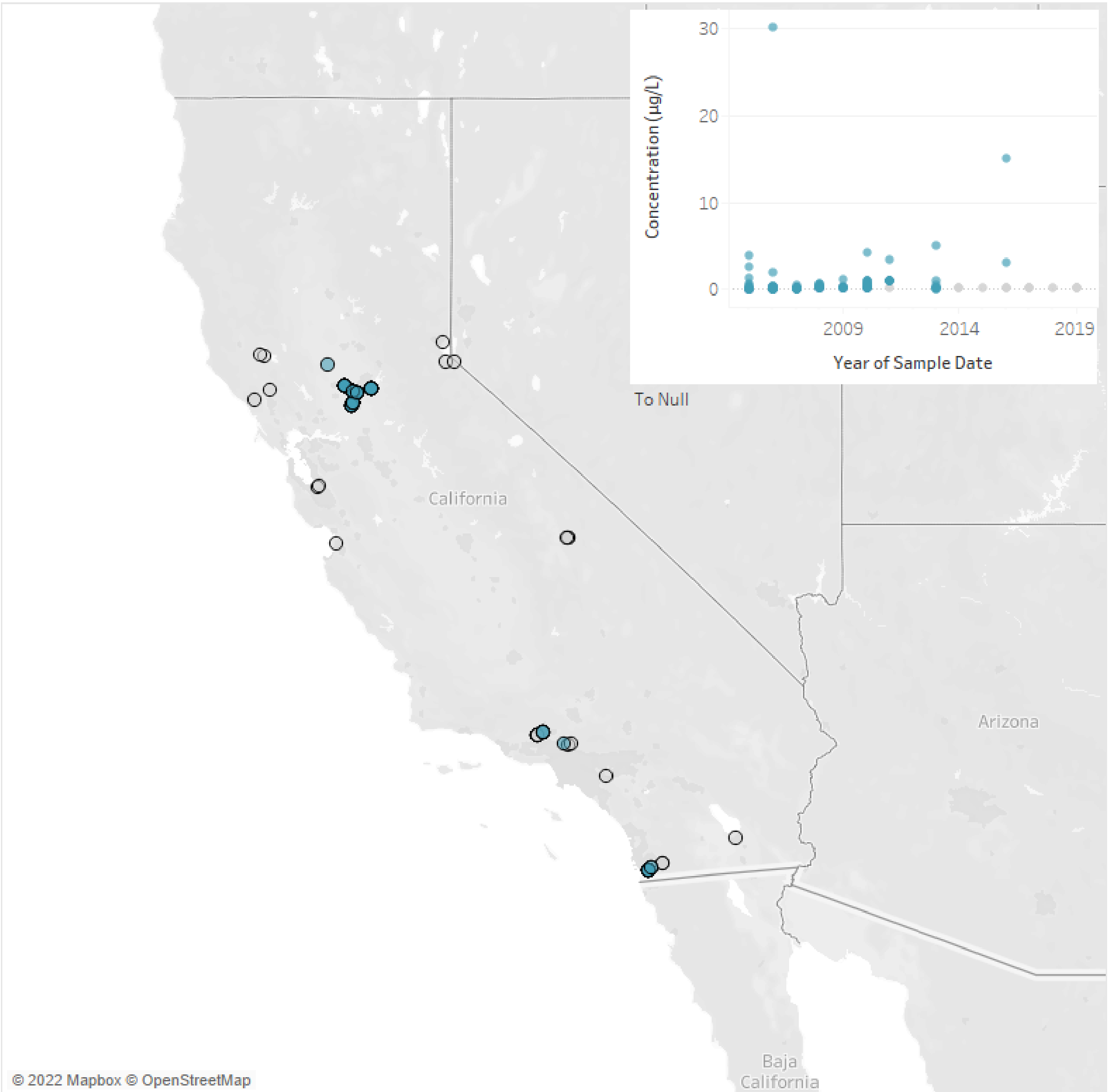


**Figure 6.2. Di-2-ethylhexyl phthalate in freshwater, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

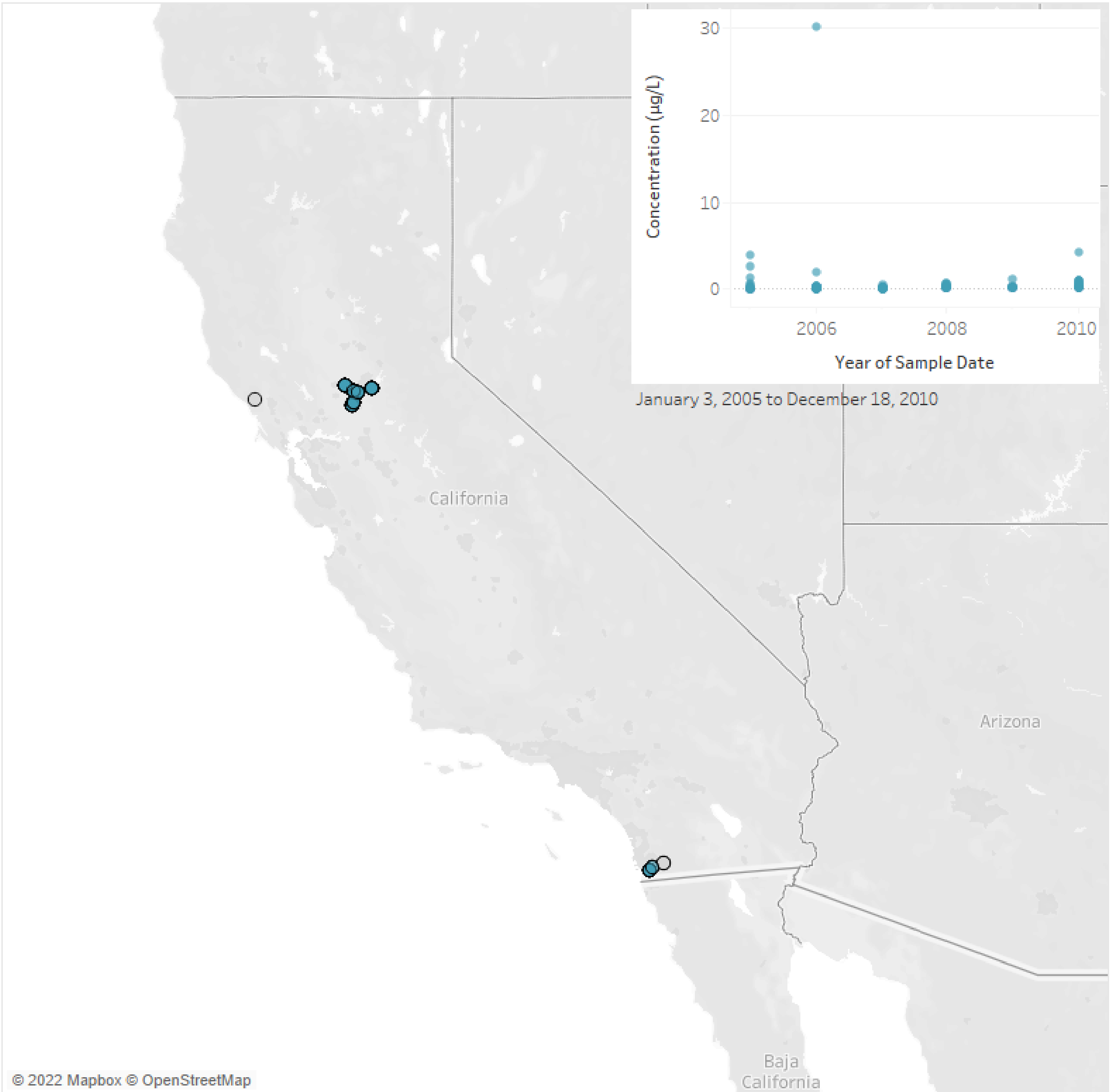


**Figure 6.3. Di-2-ethylhexyl phthalate in freshwater, 2005-2010. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

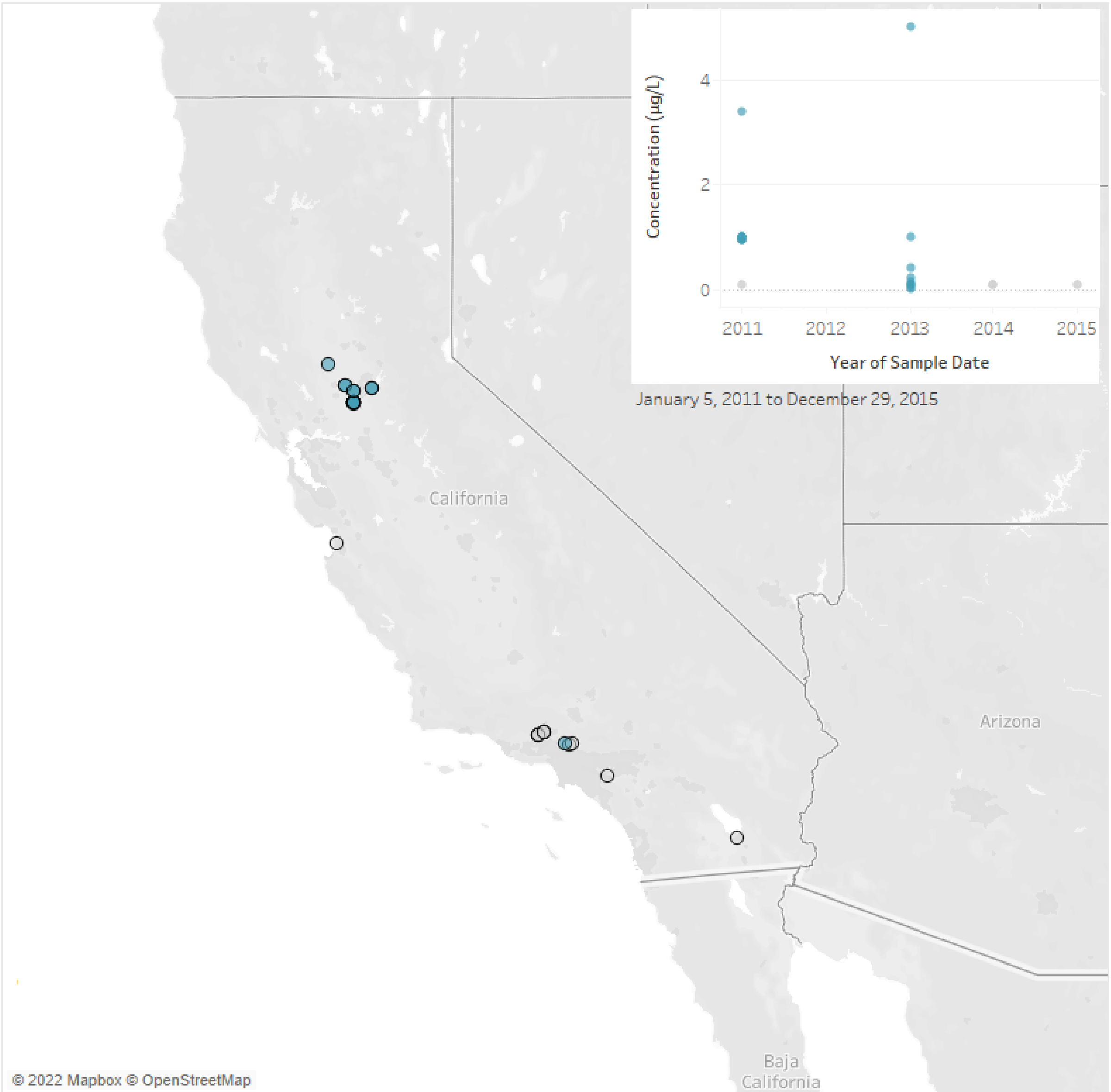


**Figure 6.4. Di-2-ethylhexyl phthalate in freshwater, 2011-2015. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

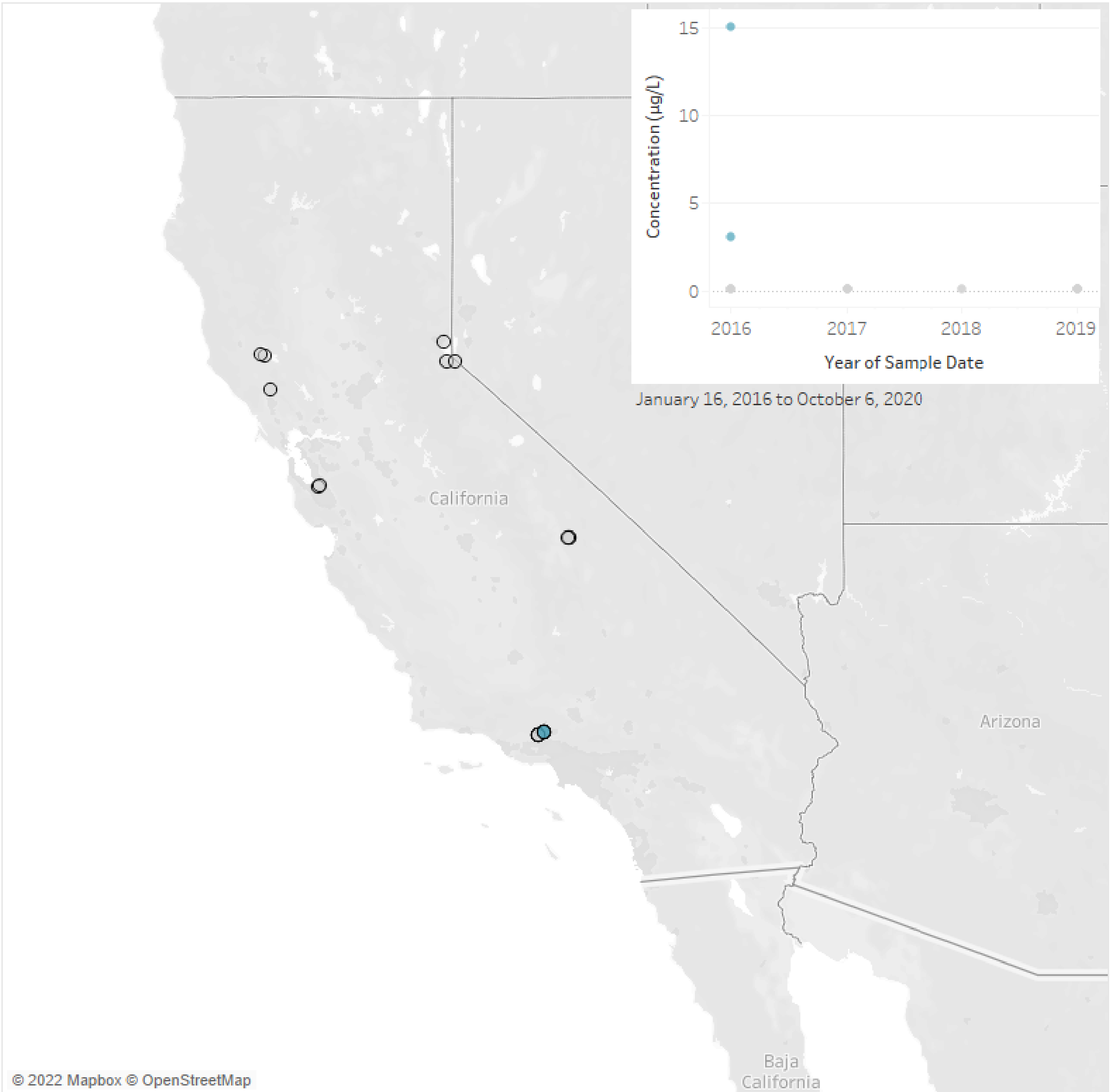


**Figure 6.5. Di-2-ethylhexyl phthalate in freshwater, 2016-2022 (data available in State Water Board dataset is through 2019). Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

Preliminary monitoring prioritization outcome

- $MTQ_{detect}$ ≤1 (0.17), trend >2.5 (2.8), N≥10 (224)
- $MTQ_{sub}$ ≤1 (0.16), trend <0.7 (0.5), N≥10 (283)
- Preliminary Monitoring Prioritization: **A3**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1)
  - Both $MTQ_{detect}$ and $MTQ_{sub}$ available and ≤1. Monitoring refinement based on $MTQ_{detect}$.
- A3 Refined Decision Framework Figure
  - Outcome based on current refined decision framework:
    - $MTQ_{detect}$ >0.1 and ≤1, N≥10
    - Spatial and temporal overlap of two most recent sampling periods (2010-2015 and 2016-2021) indicate overlap in Southern California samples based on a limited sample size (N=2) and no overlap in other parts of the state.
    - Further evaluation needed to evaluate data indicating a steeply increasing trend (2.8).

Application of the refined monitoring prioritization methodology to di-2-ethylhexyl phthalate in freshwater is an example where additional evaluation of the data, beyond that summarized in the Appendix I tables, will be necessary to determine if a steeply increasing trend is present. The reason for the additional evaluation is that the only location with spatial overlap is in Southern California. The overlap is based on two samples in the most recent time period for that location in Southern California and 25 samples collected from several locations in California during the previous time period. To determine whether a steeply increasing trend exists requires calculating the MEC for only the location with spatial overlap. The tables in Appendix I do not provide CEC concentration data on a sample-by-sample basis. If such a steeply increasing trend is present, the refined prioritization for di-2-ethylhexyl phthalate would be 'High' (A2), the same as for the preliminary monitoring prioritization. If insufficient data exist to determine trend, the refined prioritization changes to 'Low' (C4). If evaluation of the sample-by-sample data leads to a recalculation of trend and the trend is either stable or decreasing, the refined monitoring classification could change to either 'Moderate' (B3) or not a monitoring priority (D1), respectively, assuming a sample size of two detects is considered sufficient to establish the presence or absence of a trend. Regardless, this example points out some of the nuances of the monitoring prioritization process and why care needs to be exercised in its application.

### *6.2.2.3 3,4-Dichloroaniline*

The refined monitoring prioritization is based on concentrations reported for the dissolved freshwater matrix. The freshwater total matrix had relatively few samples (N<25), MTQ=0.5 and insufficient data to evaluate trends.

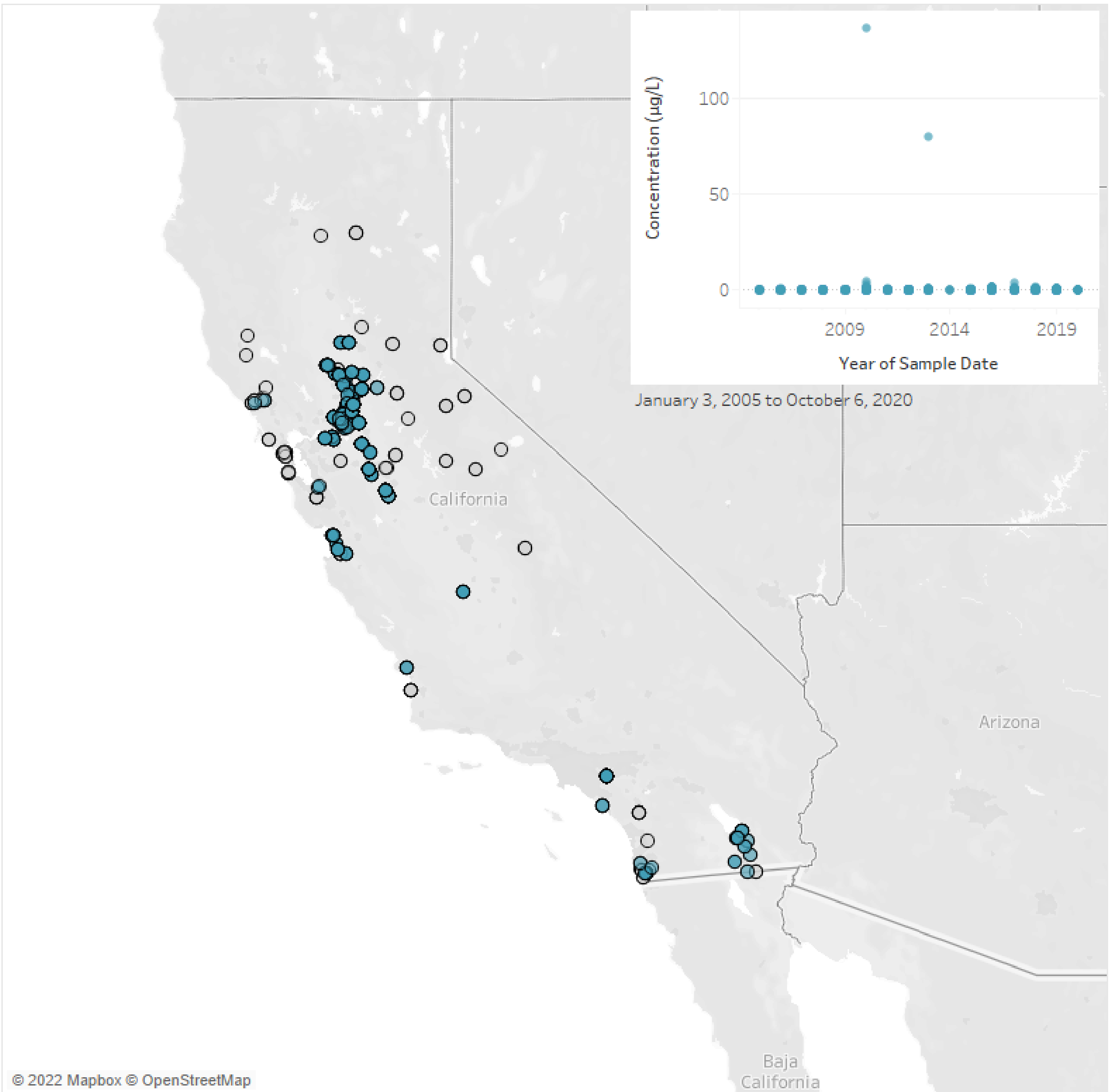


**Figure 6.6. 3,4-Dichloroaniline in freshwater, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

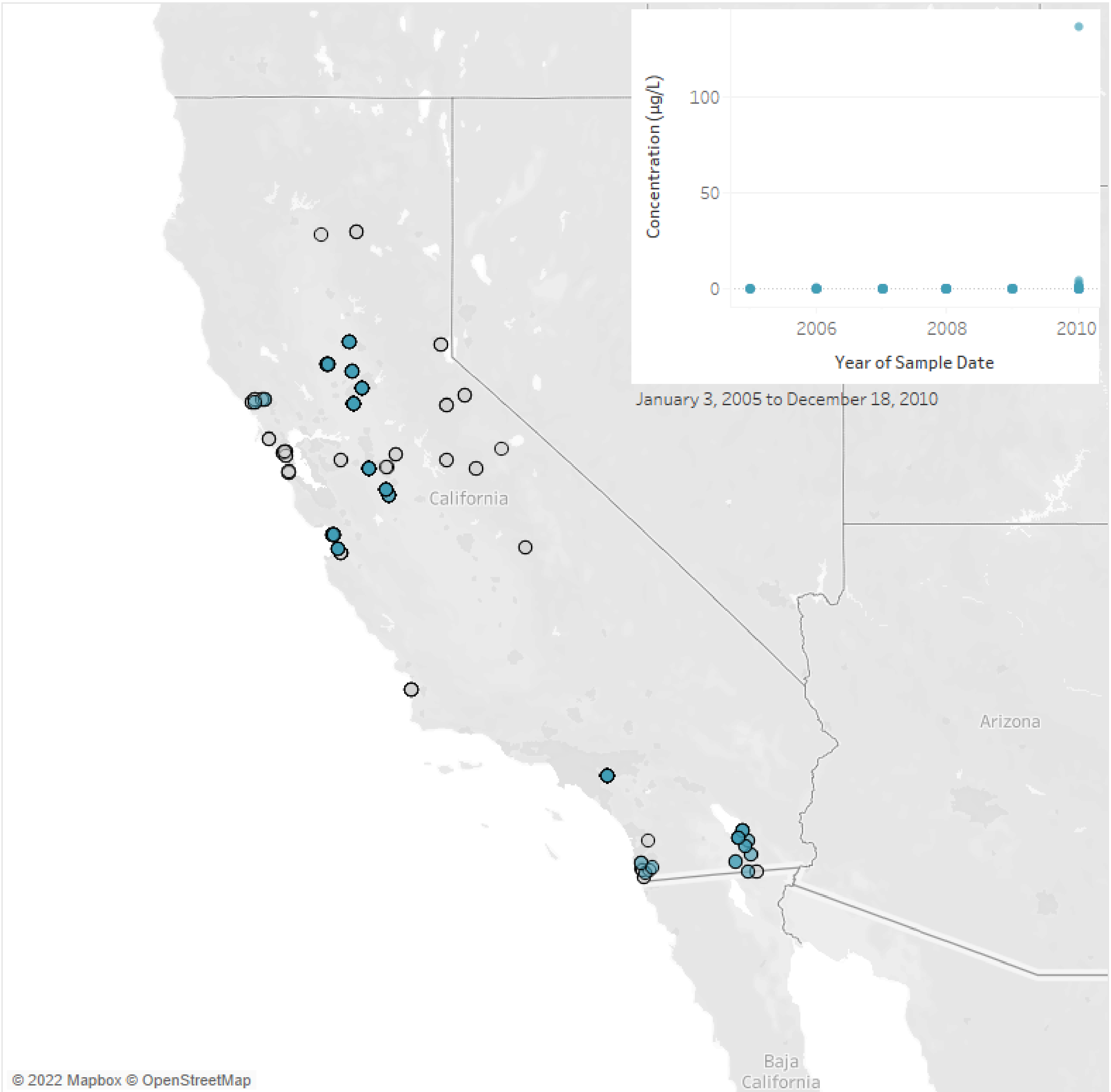


**Figure 6.7. 3,4-Dichloroaniline in freshwater, 2005-2010. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

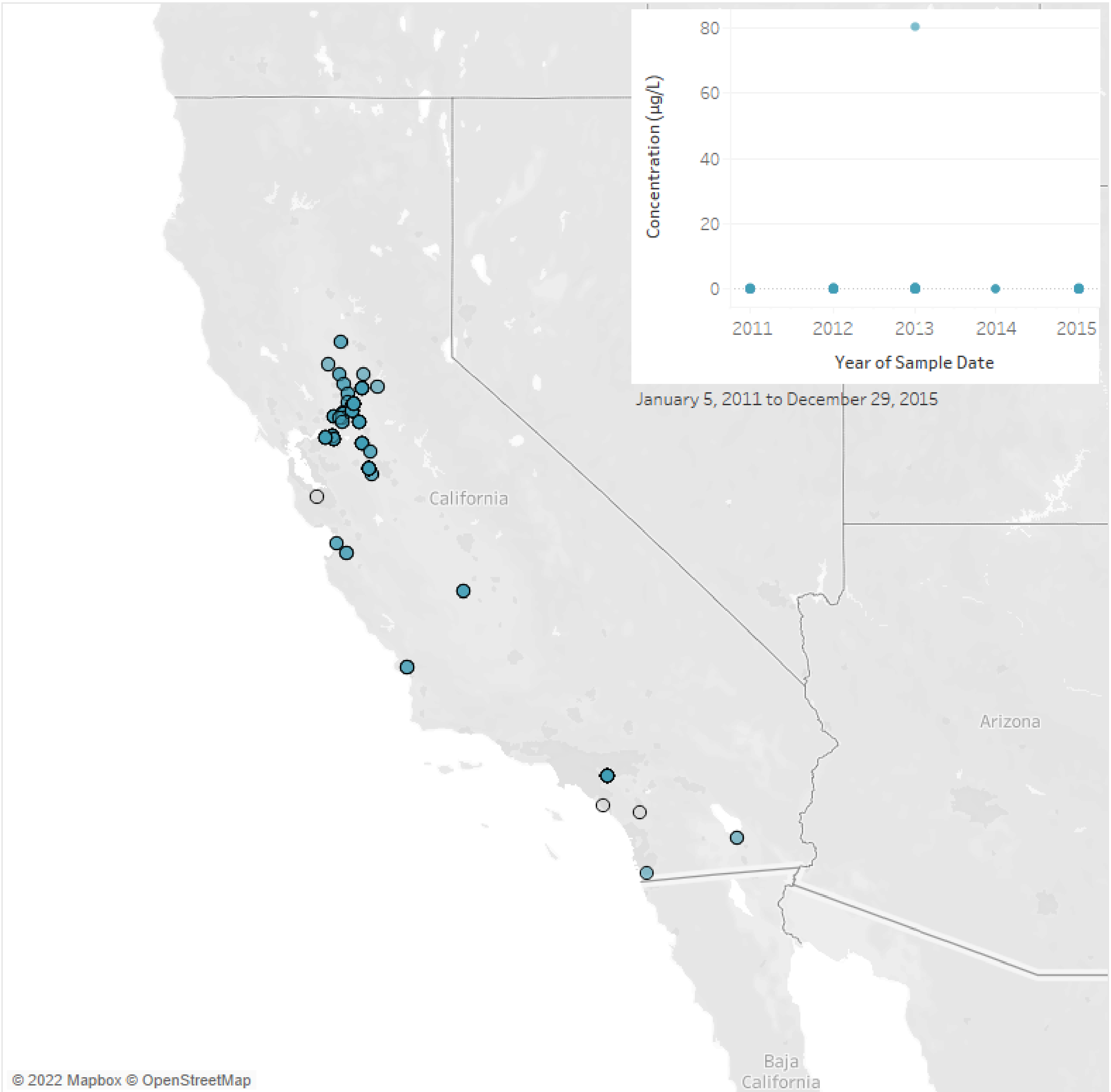


**Figure 6.8. 3,4-Dichloroaniline in freshwater, 2011-2015. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

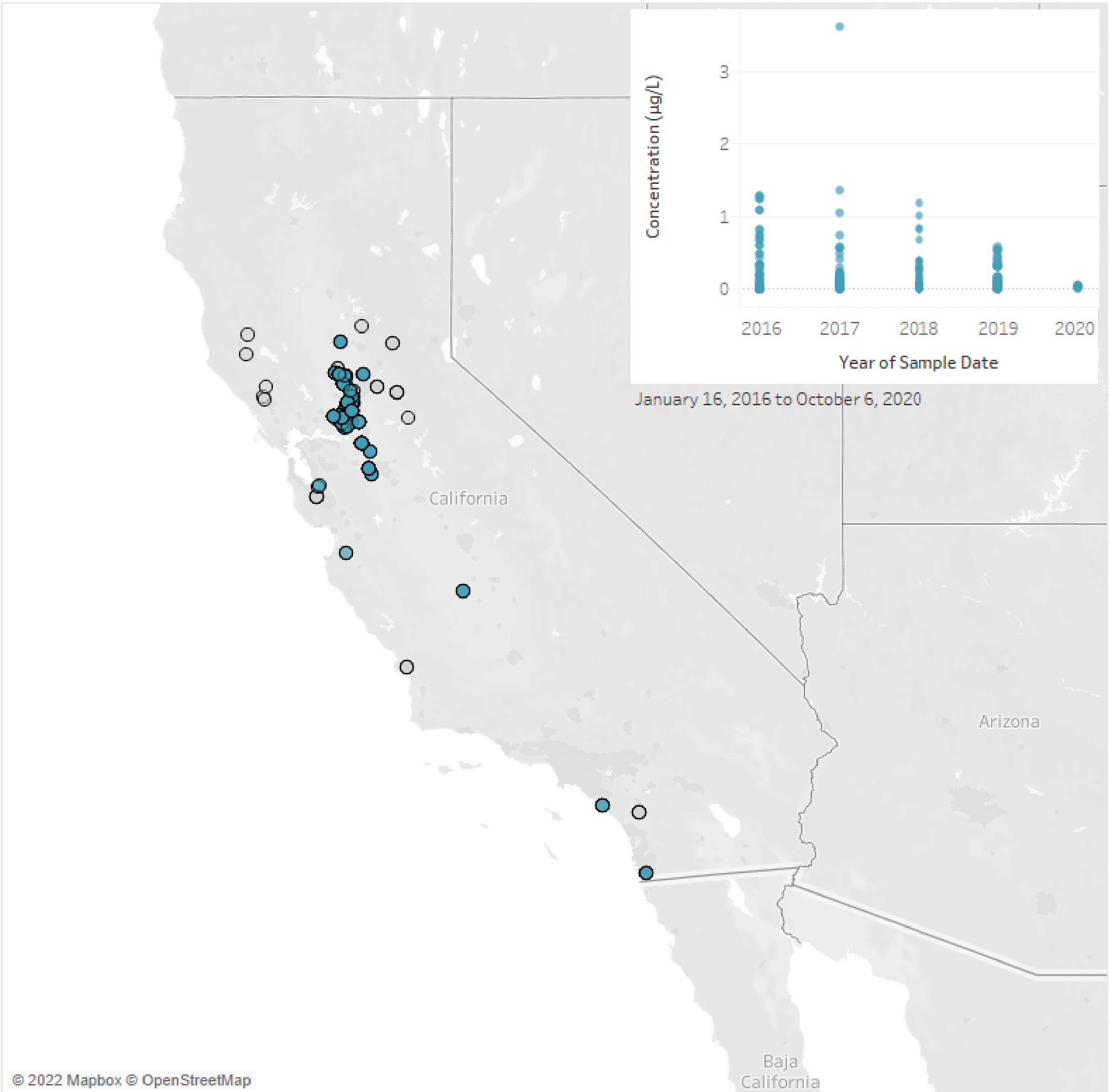


**Figure 6.9. 3,4-Dichloroaniline in freshwater, 2015-2022 (data available in State Water Board dataset is through 2019). Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

Preliminary monitoring prioritization outcome

- $MTQ_{detect}$ >10 (34), trend >2.5 (9.9), N≥10 (1034)
- $MTQ_{sub}$ >10 (19), trend >2.5 (10), N≥10 (1473)
- Preliminary Monitoring Prioritization: **A1**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1)
    - Both $MTQ_{detect}$ and $MTQ_{sub}$ available and >1. Monitoring refinement based on $MTQ_{detect}$.
- A1 Refined Decision Framework Figure
    - Outcome based on current refined decision framework:
        - $MTQ_{detect}$ ≥10, N≥10; refined monitoring priority: High (A1).

The refined monitoring prioritization of 'High' (A1) for 3,4-Dichloroaniline is the same as the preliminary monitoring prioritization.

### *6.2.2.4 Erythromycin*

The refined monitoring prioritization is based on concentrations reported for the dissolved freshwater matrix. The freshwater total matrix had relatively few samples (N=43), MTQ<0.0009, no data from the most recent sampling period and decreasing trend between the two prior sampling periods.

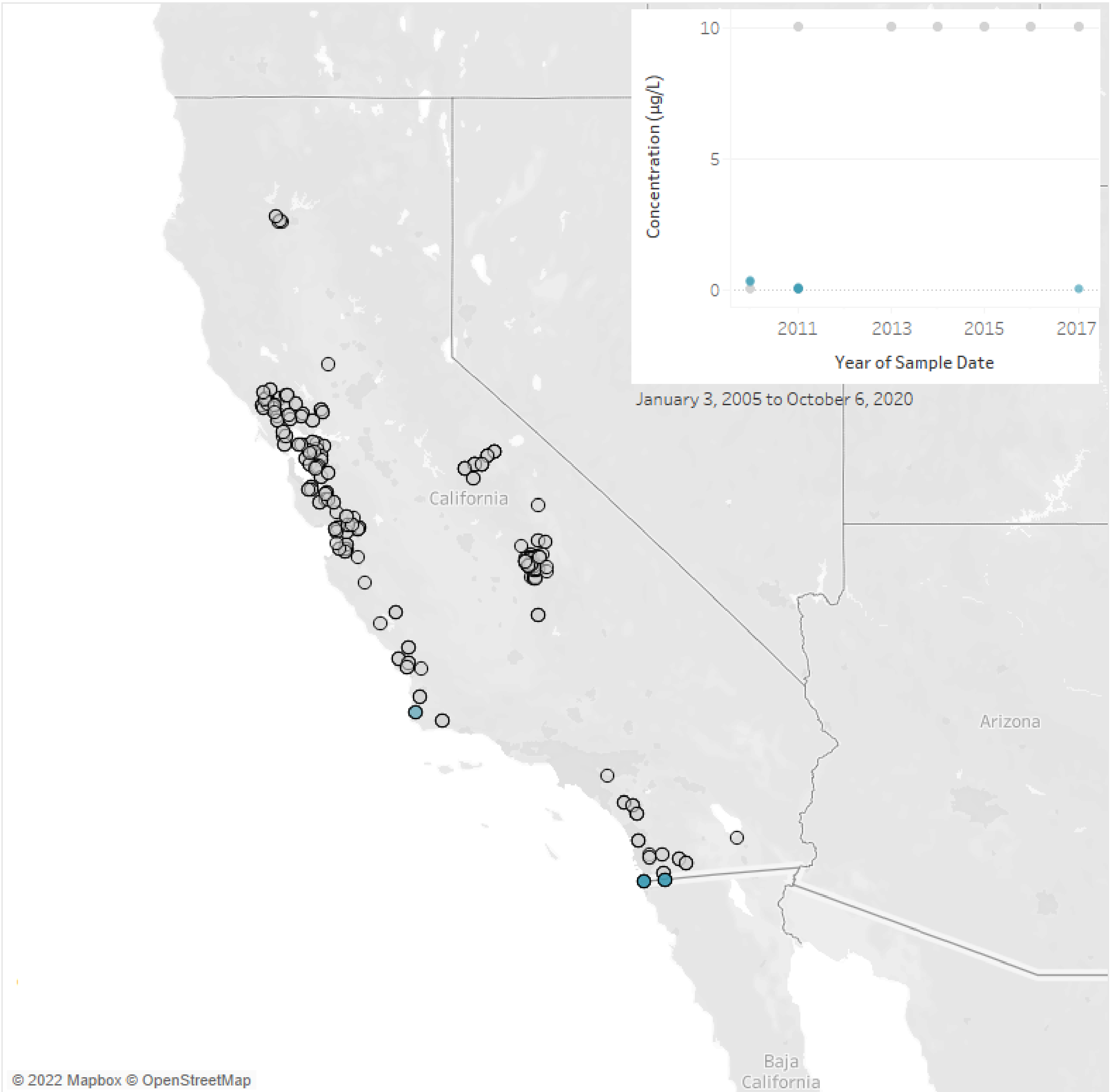


**Figure 6.10. Erythromycin in freshwater, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

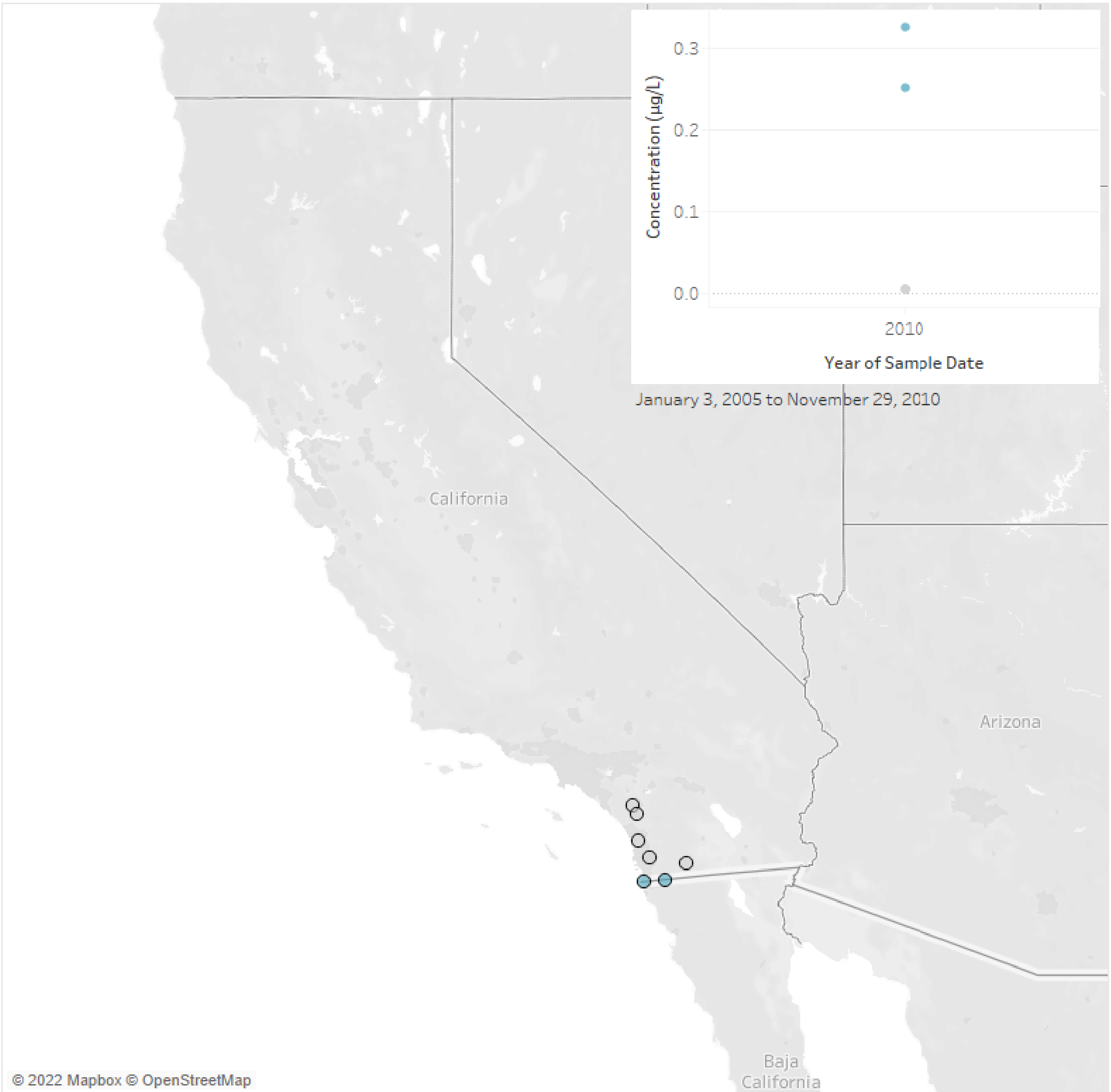


**Figure 6.11. Erythromycin in freshwater, 2005-2010. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

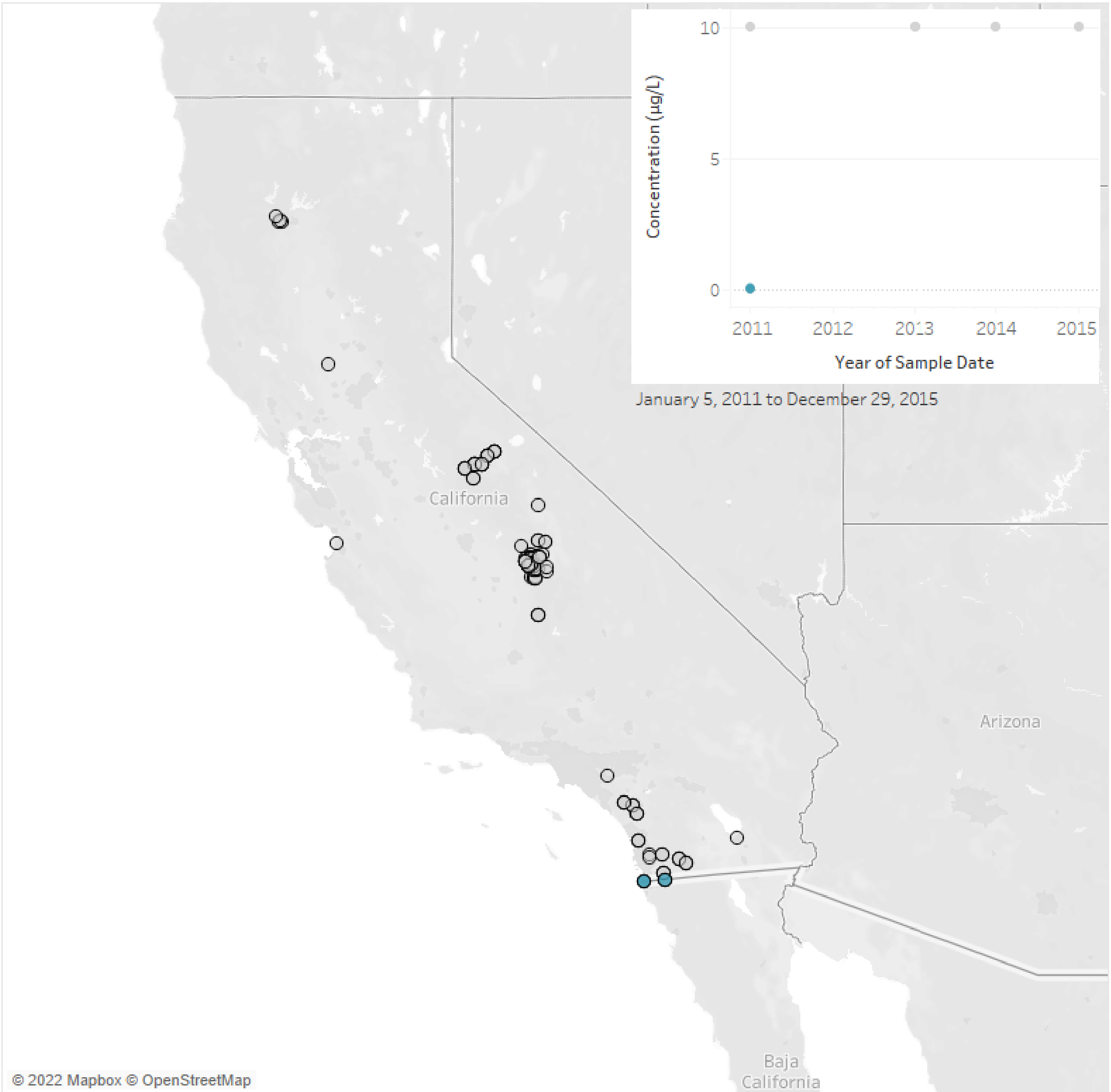


**Figure 6.12. Erythromycin in freshwater, 2011-2015. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

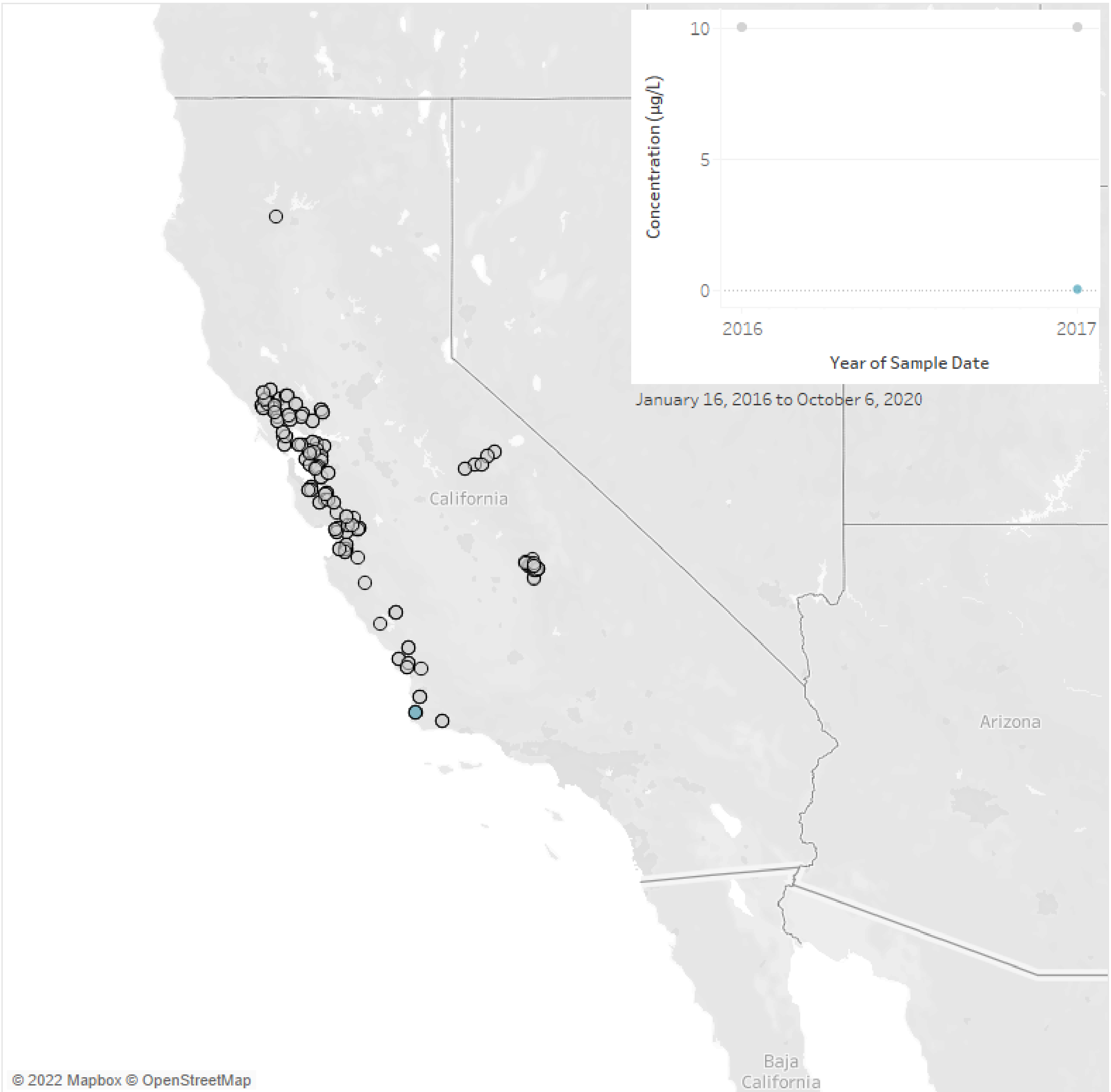


**Figure 6.13. Erythromycin in freshwater, 2016-2022 (data available in State Water Board dataset is through 2017). Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L). Depicted are a map of the state with locations from the dataset for this compound, and an inset plot of concentrations over time.**

Preliminary monitoring prioritization outcome.

- $MTQ_{detect}$ ≤1 (0.00006), trend ID (-), N<10 (1)
- $MTQ_{sub}$ ≤1 (0.03), trend >2.5 (20), N≥10 (425)

- Preliminary Monitoring Prioritization: **B2**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1)
    - Both $MTQ_{detect}$ and $MTQ_{sub}$ available, $MTQ_{detect}$ <1. Monitoring refinement based on $MTQ_{detect}$.
- A1 Refined Decision Framework Figure
    - Outcome based on current refined decision framework:
        - $MTQ_{detect}$ ≤1, N<10: Limited sample size. Special Study: Evaluate need for additional monitoring.

Based on the refined monitoring prioritization, the preliminary monitoring prioritization of ‘Moderate’ (B2) for erythromycin changes to needing additional evaluation (Special Study) to better understand variation in reported MDLs and determine whether monitoring is required given that the $MTQ_{detect}$ is less than 1 and the positive trend of $MTQ_{sub}$ appears to be driven by an increase in MDL over time.

#### *6.2.2.5 Acetaminophen*

The refined monitoring prioritization is based on concentrations reported for the dissolved freshwater matrix. The freshwater total matrix has few samples (N=2), both are non-detects resulting an $MTQ_{sub}$ =2,000 suggesting an elevated detection is driving the MTQ, and insufficient data to evaluate trend.

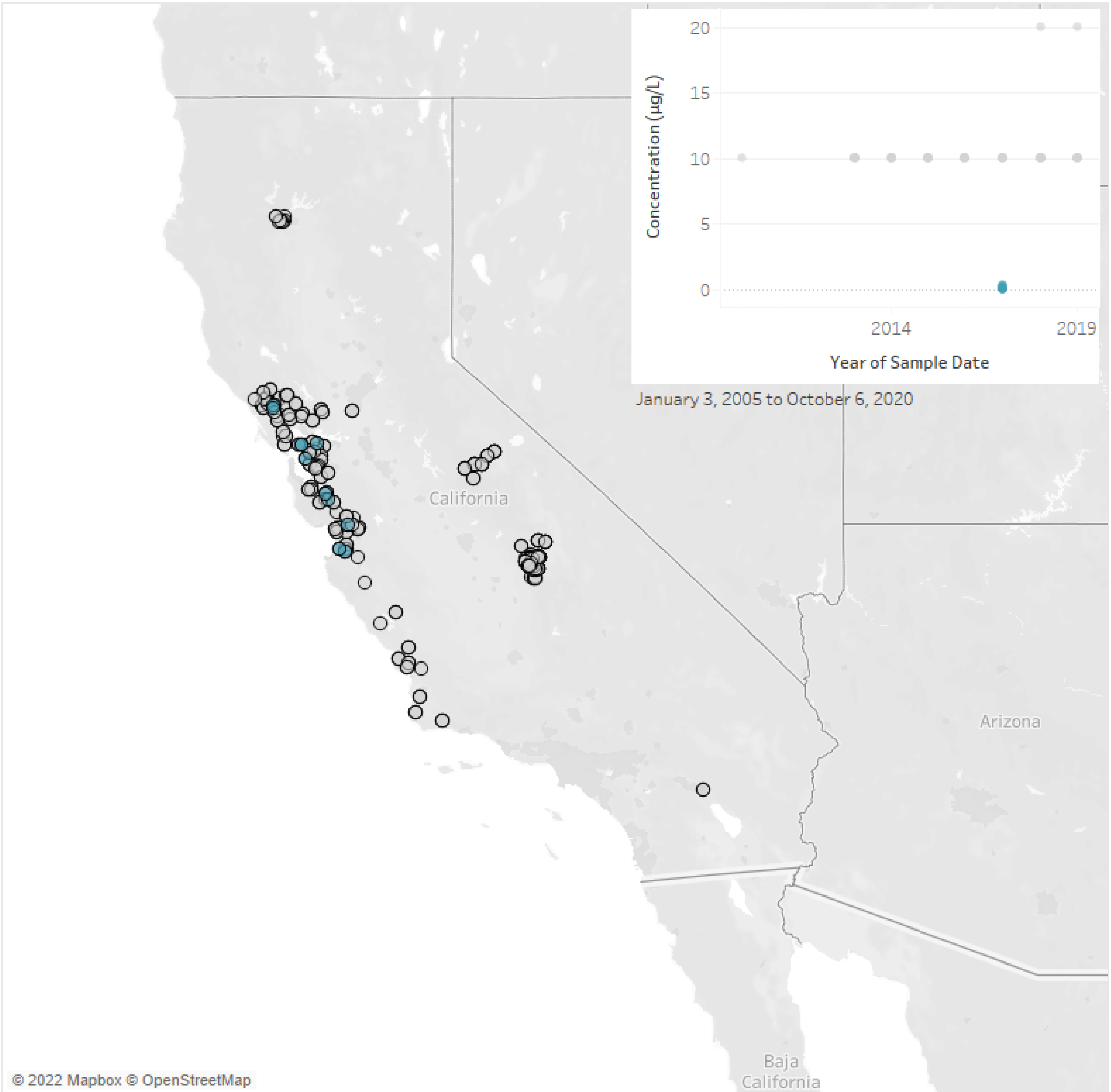


**Figure 6.14. Acetaminophen in freshwater, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**


**Figure 6.15. Acetaminophen in freshwater, 2005-2010. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

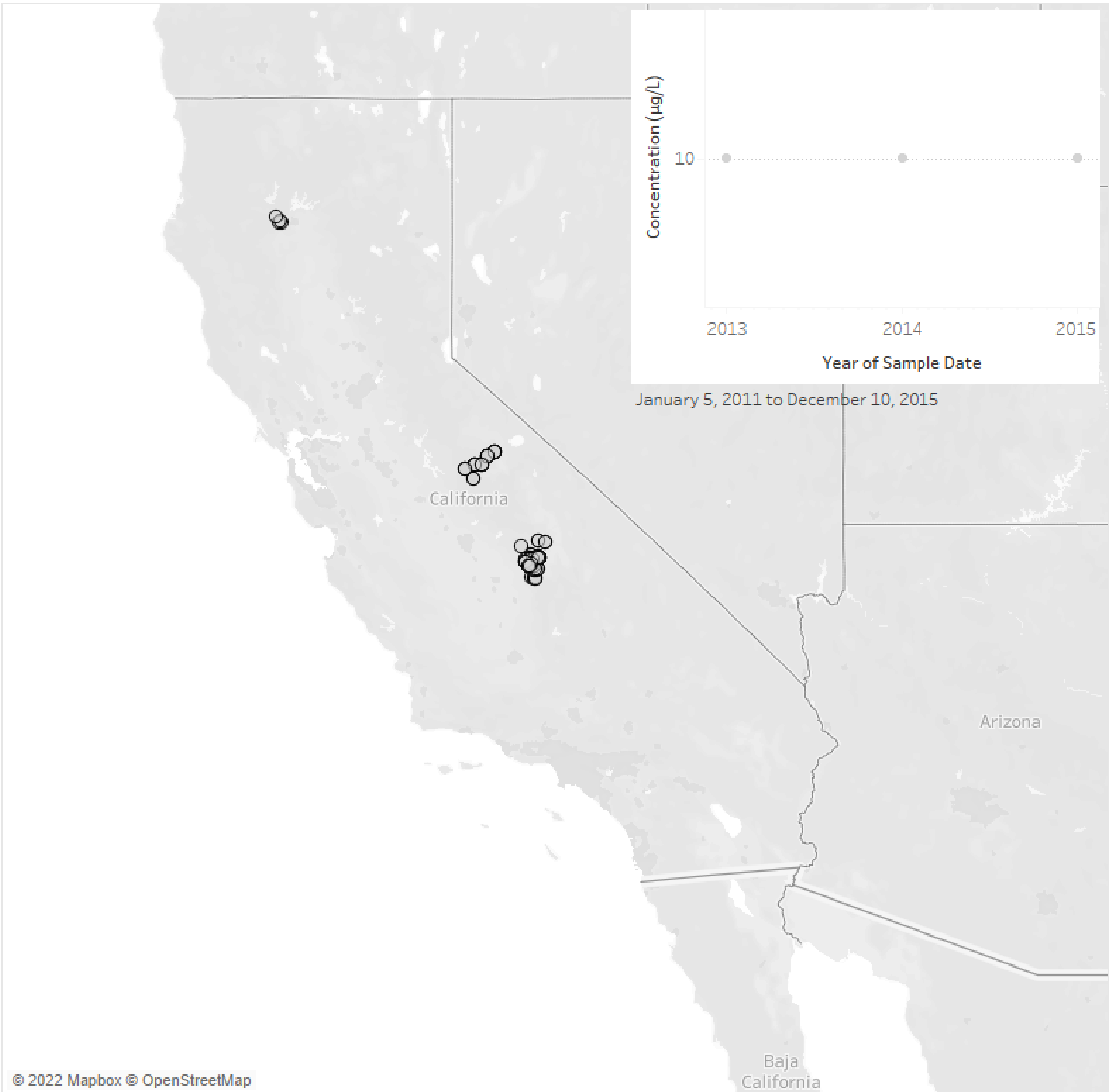


**Figure 6.16. Acetaminophen in freshwater, 2011-2015. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

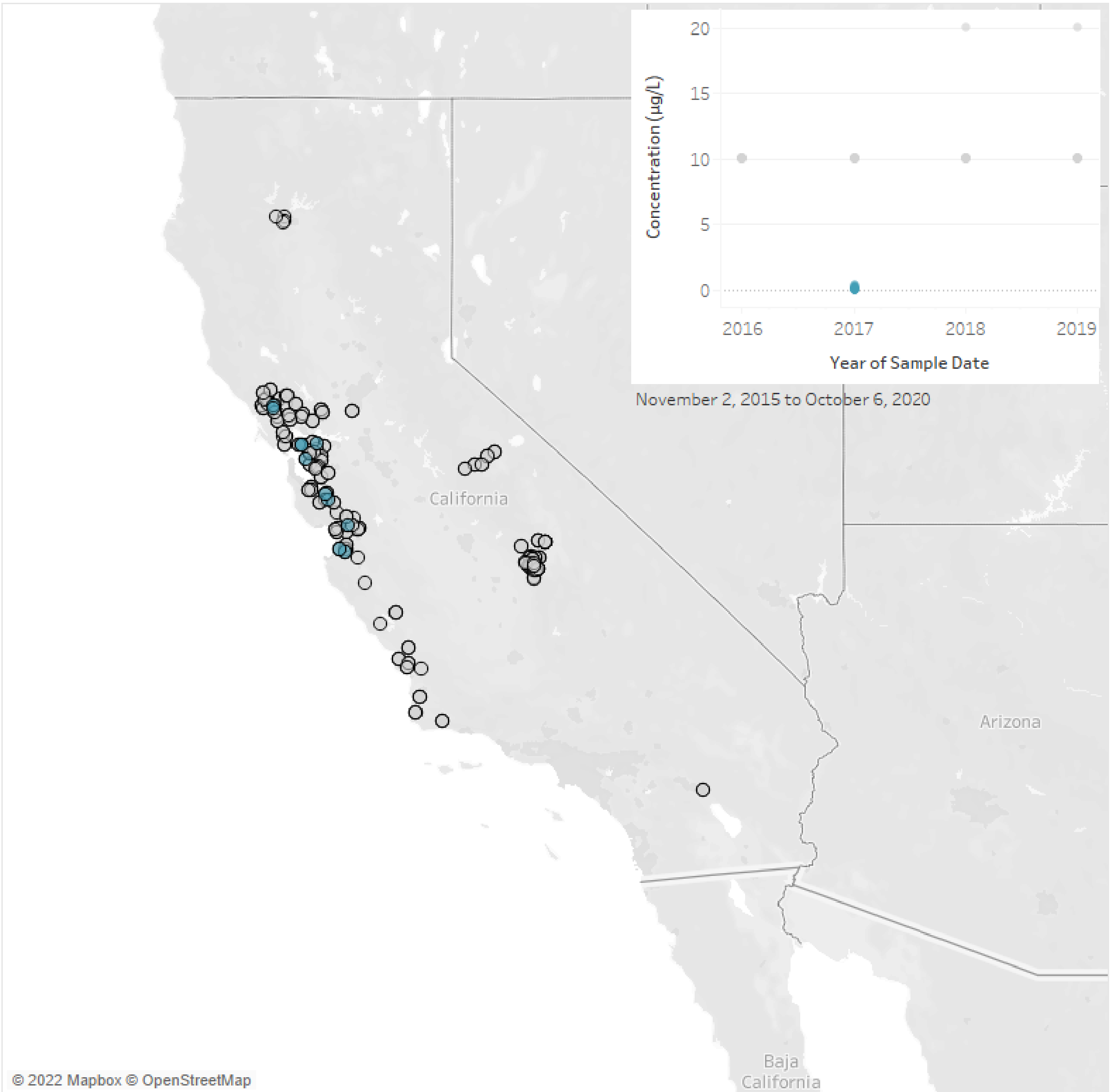


**Figure 6.17. Acetaminophen in freshwater, 2016-2022 (data available in State Water Board dataset is through 2019). Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

Preliminary monitoring prioritization outcome.

- $MTQ_{detect}$ ≥10 (23), trend ID (-), N≥10 (11)
- $MTQ_{sub}$ ≥10 (1,000), trend >2.5 (8), N≥10 (495)
- Preliminary Monitoring Prioritization: **A1**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1)
    - Both $MTQ_{detect}$ and $MTQ_{sub}$ available and >1. Monitoring refinement based on $MTQ_{detect}$.
- A1 Refined Decision Framework Figure
    - Outcome based on current refined decision framework:
        - $MTQ_{detect}$ ≥10, N≥10; refined monitoring priority: High (A1).

The refined monitoring prioritization of High (A1) for acetaminophen is the same as the preliminary monitoring prioritization. Review of the data indicates that 484 of 495 samples are non-detect and that the detection limit appears to be substantially greater than the MTL resulting in MTQs >10 even for non-detect samples. This is an example where even though a CEC has a ‘High’ (A1) monitoring priority, additional evaluation and refinement of either or both the MTL and MDL would likely be a better use of limited resources in lieu of collecting more data, the majority of which appear likely to be non-detect but with MTQs well above 1 (unity).

### *6.2.2.6 4-Nonylphenol*

The refined monitoring prioritization is based on concentrations reported for the total marine water matrix. No data were available for the marine water dissolved matrix.

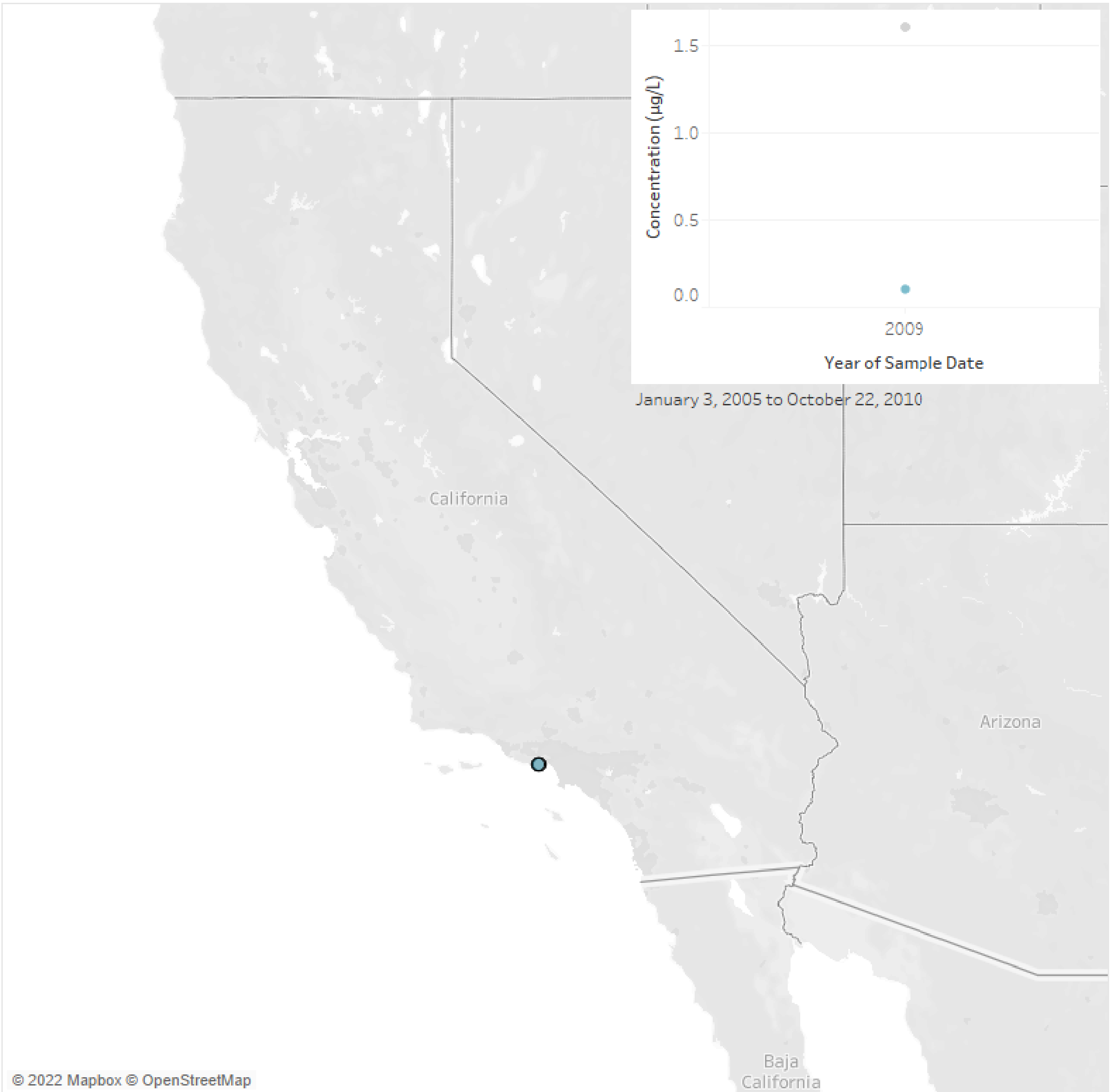


**Figure 6.18. 4-Nonylphenol in marine water, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

Preliminary monitoring prioritization outcome.

- $MTQ_{detect}$ ≥10 (1,000), Trend ID (-), N<10 (1)
- $MTQ_{sub}$ ≥10 (16,000), Trend ID (-), N<10 (6)
- Preliminary Monitoring Prioritization: **A1**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1)
    - Both $MTQ_{detect}$ and $MTQ_{sub}$ available and >1. Monitoring refinement based on $MTQ_{detect}$.
- A1 Refined Decision Framework Figure
    - Outcome based on refined decision framework (Figure G.1):
        - $MTQ_{detect}$ ≥10, N<10,
        - No spatial overlap of two most recent sampling periods given that 4-nonyl phenol was detected in only a single sample.
            - Limited sample size, special study. Evaluate need for additional monitoring.

Based on the refined monitoring prioritization, the preliminary monitoring prioritization of ‘High’ (A1) for 4-nonyl phenol changes to a special study to evaluate the need for additional monitoring. Such a special study should include review of the MTL and whether, as described in Chapter 4, dividing the 4-nonyl phenol freshwater MTL by an uncertainty factor of 10 to derive the marine water MTL is appropriate and whether the MDL can be refined such that concentrations below the MTL can be detected.

#### *6.2.2.7 Chlorpyrifos*

The refined monitoring prioritization is based on concentrations reported for the total marine water matrix. No data were available for the marine water dissolved matrix.

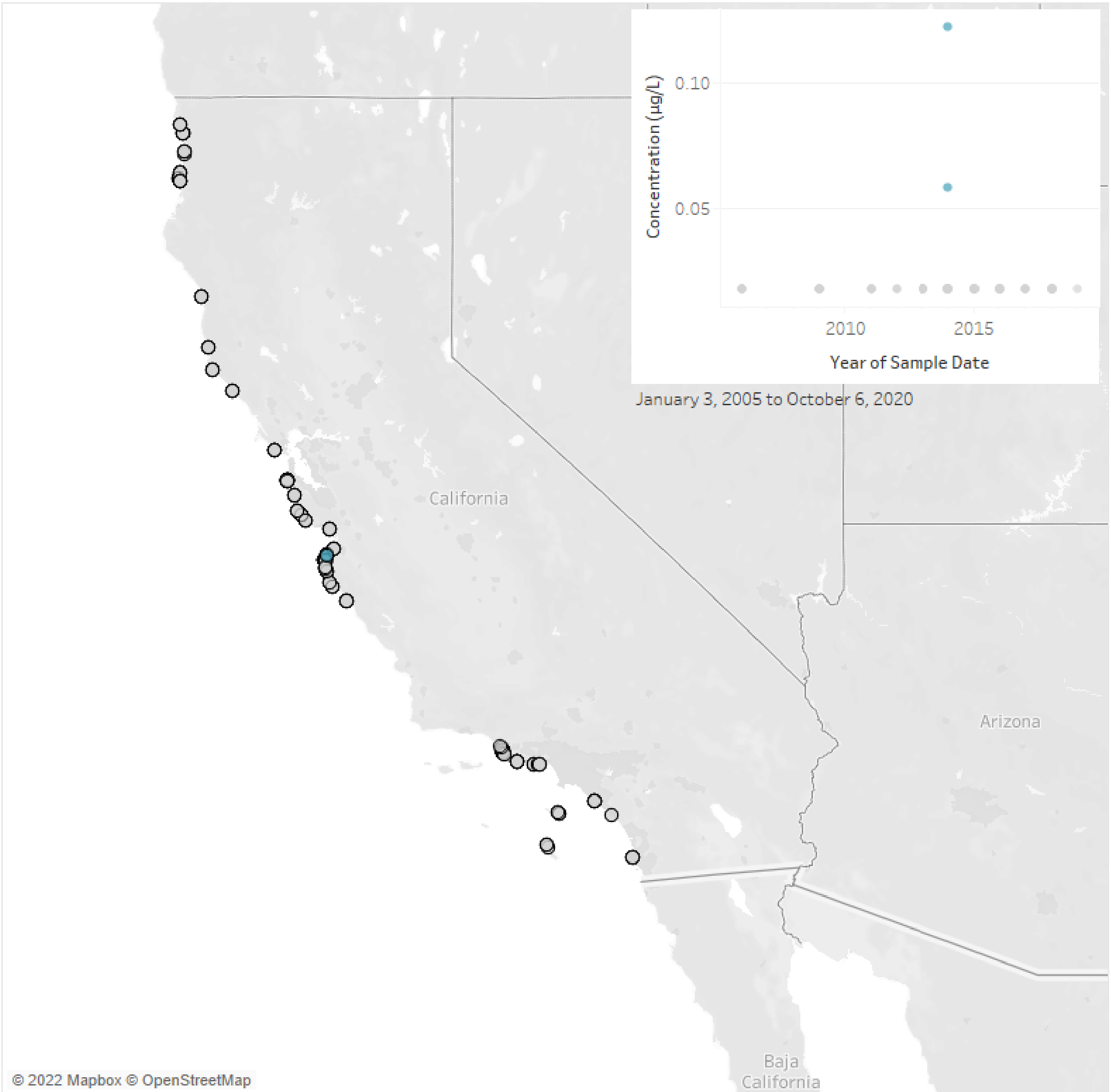


**Figure 6.19. Chlorpyrifos in marine water, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

Preliminary monitoring prioritization outcome.

- $MTQ_{detect}$ ≥10 (289), Trend ID (-), N<10 (2)
- $MTQ_{sub}$ ≥10 (45), Trend stable (1), N≥10 (656)
- Preliminary Monitoring Prioritization: **A1**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1)
  - Both $MTQ_{detect}$ and $MTQ_{sub}$ available and >1. Monitoring refinement based on $MTQ_{detect}$.
- A1 Refined Decision Framework Figure
  - Outcome based on refined decision framework (Figure G.1):
    - $MTQ_{detect}$ ≥10, N<10,
    - No spatial overlap of two most recent sampling periods given that chlorpyrifos was detected in only two samples and both samples were collected in the 2011-2015 time period.
      - Limited sample size, special study. Evaluate need for additional monitoring.

Based on the refined monitoring prioritization, the preliminary monitoring prioritization of 'High' (A1) for chlorpyrifos changes to a special study to evaluate the need for additional monitoring, paying special attention to whether the MDL can be refined given that virtually all available data from marine waters are non-detect (657 of 659 samples) and existing MDLs result in MTQs of greater than 1. Additionally, as described in Chapter 4, most marine water MTLs are derived by dividing freshwater MTLs by an uncertainty factor of 10. The application of such an uncertainty factor to the chlorpyrifos marine MTL should be reviewed.

#### *6.2.2.8 PBDE 209*

The refined monitoring prioritization is based on concentrations reported for the total estuarine matrix. The estuarine dissolved matrix had fewer samples and lower MTQs than the estuarine total matrix and a lower preliminary monitoring prioritization (Low, C1).

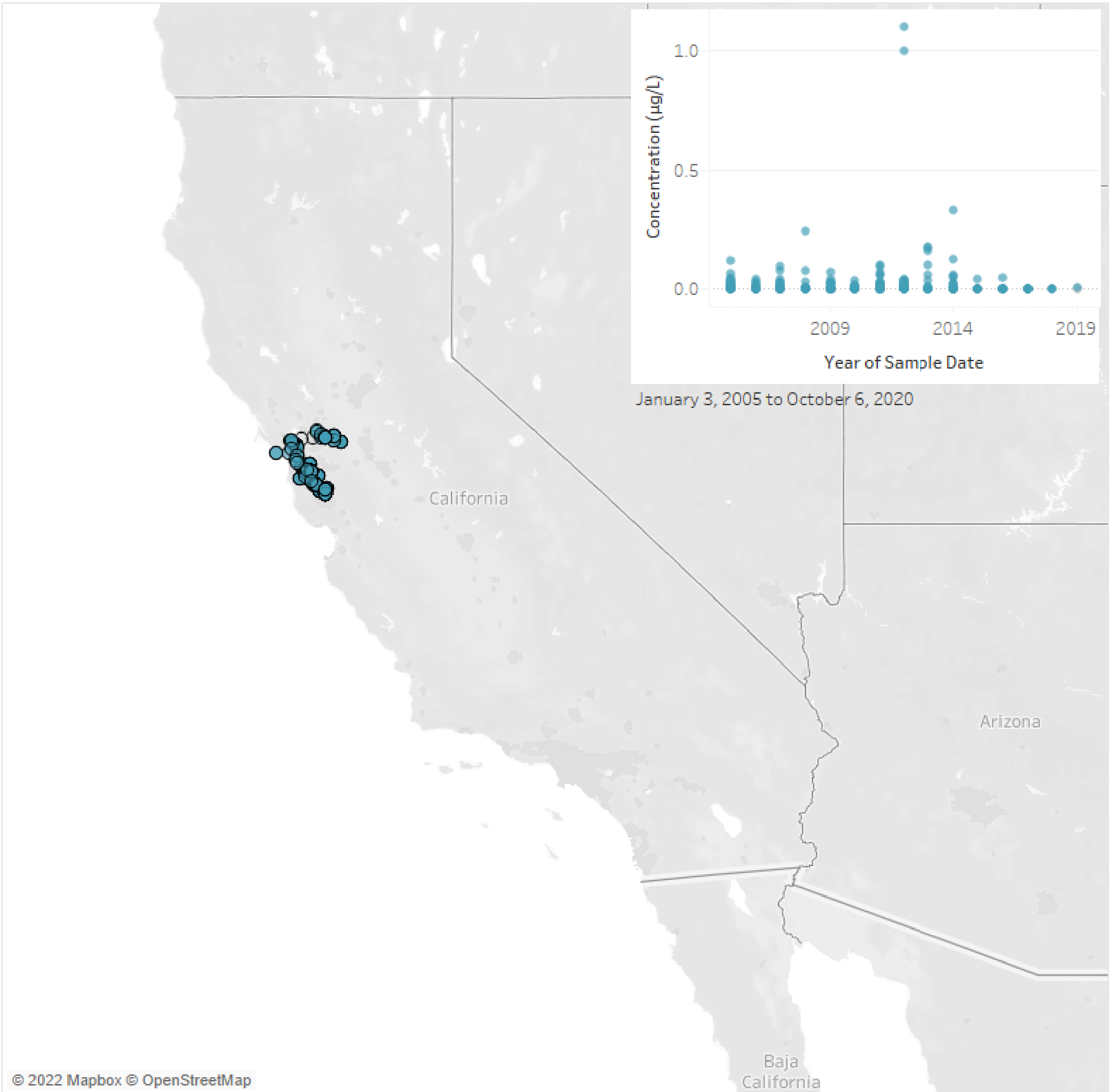


**Figure 6.20. PBDE 209 in estuarine water, all time periods. Teal symbols are detected measurements, grey symbols are non-detect measurements. Concentrations over time in inset plot are in micrograms per liter (ug/L).**

Preliminary monitoring prioritization outcome.

- $MTQ_{detect}$ ≥10 (432), Trend decreasing (0.01), N≥10 (271)
- $MTQ_{sub}$ ≥10 (315), Trend decreasing (0.2), N≥10 (377)
- Preliminary Monitoring Prioritization: **A1**

Refined Monitoring Prioritization

- MTQ Selection Table (Table 6.2.1)
    - Both $MTQ_{detect}$ and $MTQ_{sub}$ available and >1. Monitoring refinement based on $MTQ_{detect}$.
- A1 Refined Decision Framework Figure
    - Outcome based on refined decision framework (Figure G.1):
        - $MTQ_{detect}$ ≥10, N≥10: High (A1)

The refined monitoring prioritization for PBDE 209, 'High' (A1) is the same as for the preliminary monitoring prioritization. Of note is that the $MTQ_{detect}$ for the most recent time period has declined to 11 (from 432 when considering all data collected to date). As described in Chapter 4, the marine MTL for PBDE 209 was derived by dividing the freshwater MTL by an uncertainty factor of 10. Before assigning PBDE 209 a "High" monitoring priority, the applicability of the 10-fold freshwater to marine uncertainty factor should be evaluated. If it is not necessary, the $MTQ_{detect}$ would decrease to 1. If the decreasing trend is confirmed, that combined with an $MTQ_{detect}$ of 1 would result in PBDE 209 in marine water not being a monitoring priority (Out, D1). This is another example where, even though a CEC has a High (A1) monitoring priority, additional evaluation and refinement of the MTL and trend would likely be a better use of limited resources in lieu of collecting more data, the majority of which appear likely to be non-detect but with MTQs well above 1 (unity).

It should be noted that the Panel did not have the time to evaluate matrices such as sediment or biota. Completion of the prioritization with these matrices by the State Water Board is recommended, especially in light of the fact that some CECs, such as PBDEs, are persistent and will accumulate in sediment and/or biota (see Chapter 6.3).

## 6.3 Persistence and Bioaccumulation

Most of the MTLs used in the preliminary and refined monitoring prioritization methodology are based on direct toxicity to aquatic biota. Some CECs have the potential to cause adverse effects to aquatic biota and wildlife by bioaccumulating in the food web. Although not specifically included in the prioritization methodologies presented above (unless the derivation of the MTL includes effects resulting from bioaccumulation), final decisions about prioritization and inclusion in a monitoring program should account for the persistence (P) and bioaccumulation (B) characteristics of CECs.

To identify CECs that have the potential to be persistent or bioaccumulative, the Panel used criteria established by the U.S. EPA for the New Chemicals program (U.S. EPA 1999) of P > 2 months and bioconcentration factor (BCF) >1.000 (log BCF=3) for screening. These are relatively conservative criteria designed to identify problematic chemicals before manufacturing is permitted, and they serve as useful guides. The Stockholm Convention of Persistent Organic Pollutants (POPs) uses P in water of 60 days and log BCF of 3.7 as screening criteria (UNEP 2001) while the European Union uses half-life in water of 40 days and log BCF of 3.3 (European Commission 2004). BCFs and biodegradation half-lives were calculated for nearly all of the 339 CECs in Tables H.1 to H.12 using OPERA (Mansouri et al. 2018), the Quantitative Structure Property Relationship (QSPR) model available in the USEPA CompTox dashboard. In addition, the BIOWIN and BCFBAF programs in EPI Suite, the U.S. EPA package of QSAR programs (U.S. EPA 2017) were used to calculate primary biodegradation rating and BCFs, as well as biotransformation half-lives in fish, and bioaccumulation factors (BAFs) in mid-trophic level and low trophic level fish (Appendix J, Table J.1). Predicted biodegradation half-lives using OPERA were >60 days for 52 CECs while BIOWIN identified 30 CECs with primary biodegradation requiring months. The PBDE congeners predominated among the CECs with long half-life, consistent with their known behavior as POPs. In addition, the 17 PFAS In Appendix J, Table J.1 can be added to the list as they are known either to undergo little if any natural degradation, or are transformed to terminal non-degradable residues for instance perfluorooctanesulfonamide (PFOSA) to PFOS. Neither OPERA nor BIOWIN predicted the recalcitrance of the perfluoroalkyl acids as PFOS.

Sixty CECs in Appendix J, Table J.1 had predicted log BCFs and BAFs >3, the majority of which were PBDEs (50). Noteworthy pesticides and pharmaceuticals in this group included chlorpyrifos, as well as the fluorinated pesticides Fluazinam, Bifenthrin, trifluralin, and Benfluralin. However, the high priority shortlist of CECs in freshwater (Appendix J, Table T.1) only included nine compounds with predicted log BCFs > 3 (including PFNA and PFOS) although this increased to 24 if BAFs in lower trophic level fish were included (Appendix I). The BCF/BAF and persistence data would have the greatest effect on the lower priority substances (Appendix J, Table J.3) where 50 of 149 substances had BAFs >3. The P and B characteristics could be normalized and combined with MTQs to create a hazard ranking of the compounds. This has recently been done by Fang et al. (2019) who ranked 135 CECs reported in surface waters of China, the U.S. and the EU using Toxicity Priority Index (ToxPi) software by combining bioaccumulation, persistence and aquatic ecotoxicity data.

## 6.4 Designing Monitoring Programs Considering Pre-Screened CECs for Different Matrices

Based on the data contained in the State Water Board dataset, the Panel believes it is premature to recommend specific monitoring programs at this time. Before designing such programs, the preliminary monitoring priority list for fresh, estuarine, and marine waters that contain a combined 185, 133, and 48 CECs in the 'High', 'Moderate' and 'Low' priority categories, respectively, need to be refined. Further, CECs in other matrices (e.g., sediments, tissues) should also be screened and assigned a monitoring priority. Only when a more holistic view is developed of the types of CECs in the different monitoring prioritization categories, their concentrations and geographical and temporal distribution, can meaningful monitoring programs be established. The Panel envisions a range of possible CEC monitoring programs. These include:

- State-wide monitoring programs for widely distributed CECs whose MTQ is either stable or expected to increase either because concentrations are anticipated to increase or the MTL is expected to decrease;
- Local or regional monitoring programs for CECs known or expected to occur in specific geographical areas;
- Special studies for CECs with information gaps identified by the monitoring prioritization process and for which filling those gaps could have a substantial effect on that CEC's monitoring prioritization;
- Other types of monitoring programs, such as those for bioanalytical or NTA approaches, and those for receiving water.

# 7. CEC Panel Summary of Key Findings

The State Water Board and Ocean Protection Council reconvened the CEC Science Advisory Panel for Aquatic Ecosystems (Panel) to review the occurrence, relevance, and quantification of CECs in fresh, estuarine, and oceanic water bodies of California. The goal of this assignment was to provide recommendations for development of a monitoring program for CECs in various water bodies of California in support of the State's CEC program. This review built upon the previous assessment report of the Expert Panel regarding recommendations for a CEC monitoring strategy in California from 2012 (Anderson et al. 2012). In 2012, the Panel provided a conceptual approach that focused on the universe of possible CECs, considered their likely sources and fates, and adopted a risk-based tiered screening framework to identify CECs that had the greatest potential to pose a risk to the State's ecological resources and inhabitants. The main driver for updating the CEC screening process that was presented in the 2012 report is the existence of a decade or more of California-specific monitoring data as well as the exponential increase of information regarding CECs in the aquatic environment from other national and international sources. The following sections summarize the Panel's key observations and findings while preparing this review.

## 7.1 High-Level Assessment of State Water Board Dataset and Refinements and Updated Risk-Based Screening Approach

The Panel conducted a critical review of the currently available CEC dataset initially compiled by the Aquatic Science Center (ASC) for the State Water Board from public databases with California monitoring data (i.e., CEDEN, Water Quality Portal, SDWIS, CIWQS, Geotracker). Occurrence data for CECs recorded in the State Water Board dataset and published peer-reviewed literature was assembled for the ASC report (Sutton et al 2022). The CEC dataset included over 427,000 records from fresh, estuarine, and marine water ecosystems for over 420 CECs. This CEC dataset represents a major increase in available monitoring data. Several broad observations include: 1) data are available throughout California (see Chapter 2), 2) a large majority of the data are non-detects lending some support to relieving environmental concern, and 3) monitoring where frequent non-detect data are available allows for focusing resources on other locations and CECs. However, significant issues remain regarding the quality of the data (see Chapter 2.1.1) which hampers interpretation.

A full description of the occurrence dataset and the challenges associated with editing it are provided in Chapter 2.3 of the ASC report. State Water Board staff has developed code in partnership with the Panel to automate the risk-based screening approach. The State Water Board would be able to periodically pull new CEC monitoring data from these data systems to refresh the CEC dataset and risk-based prioritization, as needed.

Although the data are already publicly available, the Panel recommends making the compiled CEC dataset publicly available on the CEC Program website once the State Water Board staff have conducted the data quality review (see Chapter 7.2 below).

The review by the Expert Panel of the State Water Board dataset identified the need for several data quality refinements to resolve discrepancies within the information entered in the current dataset, as noted in the 2012 Panel report (Anderson et al. 2012). Having blanks, replicates, recovery, and other information for both targeted methods and particularly for NTA is vital. Specific aspects noted by this Panel include clarifying environmental matrix, deleting duplicate records, records without consummate data and MDLs, and assuring proper units of measurements and then applying two additional data selection criteria (i.e., number of samples and detection frequency) to improve the utility and representativeness of the data contained in the existing statewide databases.

Given the large amount of available data and the resultant time associated with the dataset cleanup, the Panel refocused on a conceptual framework demonstrating, as a “proof of concept”, an updated risk-based screening approach for the State Water Board staff to implement. This model provides three features:

- an initial prioritization of CEC compounds of interest (‘preliminary monitoring screening’),
- an approach to further narrow with priorities based on data availability, data quality, and spatial and temporal analyses (‘refined monitoring screening’), and
- additional programmatic recommendations for the State Water Board staff to move forward

The latter two features evolved from lessons learned while applying the initial prioritization scheme to 450,000 records which produced a long list of monitoring priority CECs, either High, Moderate, or Low priority, for fresh, estuarine, and marine waters. This two-step screening process and updated approach is described further in Chapter 7.1.4 below.

### 7.1.1 Updated data availability of CEC MECs

Currently the updated CEC dataset contains approximately 427,000 records in the following environmental matrices: sediment, and fresh, marine and estuarine water. Roughly 10% of the data cannot be used because they are reported as non-detects without any information to estimate or interpret an MDL. Of the usable data, roughly 23% were detected and the remainder are non-detects. Thus, roughly 400,000 data records are considered trustworthy and available for estimating MECs, although data without geographical coordinates or site information (27%) limited the utility of some of this data.

A total of 423 CECs were reported for all environmental matrices (Table 7.1). These CECs were categorized into eleven classes: pesticides, pharmaceuticals, alkyl phenols/alkyl phenol ethoxylates (AP/APEs), phthalates, polybrominated diphenyl ethers (PBDEs), brominated flame retardants (BFRs), per- and polyfluoroalkyl substances (PFAS), personal care products (PCPs), bisphenols, organophosphate esters (OPEs), and natural toxins (microcystins and marine toxins). The total records for CECs analyzed in different matrices included:

- Surface waters – ranged from 8,880 in estuarine waters to 280,653 in freshwater. These represented results from 3,622 sampling stations. The sampling years for fresh, estuarine, and marine water ranged from 2005 to 2021 with the largest number of records from 2017.
- Sediments – ranged from 15,871 in estuaries to 61,245 in freshwaters.
- WWTP – Influent, effluent and biosolids included 75,468 analyses. The majority of records are for WWTP effluents.
- Stormwater – 31,105 records.
- Biological – 25,082 records with marine biota constituting the largest group. Bivalves and fish were major sample matrices in marine and estuarine waters while results for fish predominated in freshwater records.

Pharmaceuticals constituted the largest group of individual CECs in freshwater (108) and estuarine waters (83), although only five were reported in marine waters. Pesticides were the next largest group ranging from 44 compounds in marine water to 108 in freshwater. PBDEs were the third largest group in water due to reporting for 51 congeners. Highest detection frequencies for PBDE in freshwaters were for congeners 15, 28, 47, 49, 99, 100, 119, 140 and 153). Summary data for each CEC (arithmetic mean, standard deviation, minimum, maximum as well as 25$^{th}$, 50$^{th}$, 75$^{th}$ and 90$^{th}$ percentiles) were calculated using all the results including those with detection limit substituted with a median MDL.

<u>Data Detection Frequency:</u> Overall detection frequencies for CECs in surface waters ranged from 12% in freshwater to 30% in marine waters. However, at the level of individual CECs, detection frequencies actually ranged from 0 to 100%. **Thus, a significant portion of the monitoring data were non-detects** (Table 7.1). Further complicating the records, detection limits for individual analytes often spanned several orders of magnitude or were listed as zero or left blank. Various approaches to

substitution of non-detect data were considered by the Panel and the median MDL for a specific CEC for the applicable sampling period was chosen. The 90$^{th}$ percentile value is inclusive of existing values, rather than an interpolated number. This substitution was made only for a given analyte and matrix and where at least one result above the MDL was available.

**Table 7.1 Summary of constituents of emerging concern (CECs) recorded and detected, and measured environmental concentrations (MECs) at various method detection limits (MDLs), in the State Water Board dataset. Nondetects are ND.**

| | Freshwater | Estuarine | Marine | Not recorded |
|---|---|---|---|---|
| # of records | 280653 | 21385 | 8880 | 116193 |
| # CECs detected | 257 | 201 | 99 | |
| # CECs all ND | 87 | 128 | 48 | |
| $MEC(med)_{sub}$=median MDL | 235 | 120 | 47 | |
| $MEC(min)_{sub}$=min MDL | 118 | 35 | 21 | |

The impact of substitution of the median MDL on the 90$^{th}$ percentile results was greatest for pesticides, pharmaceuticals, and PCPs in freshwater samples where 47% to 80% of 90$^{th}$ percentiles were more than 10-fold higher than the value based only on measured results. Substitution of the median lowered the 90$^{th}$ percentile by more than 10-fold in a more limited number of pesticides (10 of 99 in freshwater; 4 of 43 in estuarine water).

Substitution of the median MDL reduced variability associated with censoring the data; however, it clearly introduces uncertainty about the true range of concentrations in ambient waters. In the future, a more robust data entry process is needed to screen out, for instance, MDLs that are orders of magnitude higher than the median MDL by built-in quality checkers, such as not allowing upload of such data to databases in the first place. Guidance is also needed for monitoring programs to achieve, when necessary, lowest practical detection limits (which may be depending on the Data Quality Objectives of the study) for CECs to avoid, as much as possible, a high proportion of "less than" values. Such guidance may be dependent on the presence of other data e.g., if MTLs are known, methods should be able to measure reliably below the toxicity threshold, but do not necessarily need to measure at the limits of known technology if that is well below the threshold. Guidance may also need to be pragmatic, e.g., MDLs at half the MTL if that is meaningful. These would need to be handled on a case-by-case basis.

*Additional CECs not in the State Water Board dataset*

In addition, the Panel relied on a narrow literature review focused on potentially "new" emerging CECs. The Panel included results from peer-reviewed articles for studies of CECs in surface waters in California that were not reported in the State Water Board CEC dataset. Several of these studies utilized non-target analysis to screen extracts of surface waters. The Panel also relied on the German Environment Agency database for pharmaceuticals in surface waters, selecting reports for the USA and Canada. This yielded 133 chemicals with MECs. Tentative MTQs could be derived for 110 compounds of which 21 had MTQs >1.

### 7.1.2 Updated Toxicity Endpoints (MTLs)

Similar to an increasing number of studies reporting CEC occurrences in the aquatic environment, there is a growing body of literature regarding toxicological effects of CECs affecting a range of endpoints. Many toxicity values included in the State Water Board CEC dataset are 'Predicted No Effect Concentrations (PNECs)', derived using various methods and uncertainty (safety) factor assessments. Uncertainty/safety factors are used to ensure precaution and add conservatism when determining thresholds for toxicity or adverse effects. In many cases, PNECs included these uncertainty/safety factors, but do not provide the rationale for their inclusion. Since the transparency and rationale was often unclear, the Panel removed the uncertainty safety factors when provided and used the data from the acute or chronic toxicity study listed. Uncertainty/safety factors were then applied based upon the expertise of the Panel. The safety factors employed attempted to provide conservative measures of toxicity for compounds that had limited chronic/reproduction data, had endocrine modes of action, or had freshwater toxicity values, but not saltwater toxicity values. Thus, the Panel attempted to reduce the uncertainties associated with values from other databases where there was limited data.

The Panel used several toxicity databases to determine toxicity values. Briefly, toxicity endpoints for roughly 400 compounds (identified from the State Water Board CEC dataset) were tabulated into a compiled toxicity dataset with values derived from the U.S. EPA in the form of Aquatic Benchmark values for pesticides, the Computational Toxicology (CompTox) Database and NORMAN Database for other compounds. In general, preference was given to U.S. EPA Aquatic Benchmarks (for pesticides) and CompTox data with subsequent use of the NORMAN Database if the compound was not found in either of the U.S. EPA databases. The following is a summary of the Panel's key assumptions for developing MTLs.

- Selection of toxicity endpoints – The lowest toxicity value available for an aquatic species was selected for the MTL. Toxicity values for terrestrial plants (e.g., lettuce) were not selected for the MTL development. If the lowest value available was an acute endpoint, an acute:chronic safety factor was applied (lowest acute value/10). Exception was given to reproduction studies which was always considered a chronic effect, even though the duration of exposure was often acute. In those cases, the acute:chronic safety factor was not applied. Ten-fold safety factors were also applied if the U.S. EPA CompTox database indicated a significant endocrine disruption identification, or the literature showed significant endocrine effects for the compound.

- Marine or Estuarine water MTLs – For this initial prioritization, marine and estuarine MTLs were derived by dividing the freshwater MTL by a 10-fold safety factor. The Panel recommended for future use that endpoints from marine species which are present in some instances in the USEPA CompTox or NORMAN databases be prioritized. In addition, peer-reviewed literature could also be utilized to derive MTLs for marine and estuarine environments.

- Pesticide MTLs – U.S. EPA Aquatic Benchmark data were used. In general, toxicity values were presented as acute or chronic responses in either plants/algae, invertebrates, or fish. Generally, the lowest chronic toxicity value of the species was targeted for MTL derivation. If an acute value was lower than the chronic value, the acute value was used without acute:chronic safety factor addition. An additional 10-fold safety factor was applied if the compound was determined to have significant endocrine disrupting potential.

- Use of NORMAN database – the lowest PNEC tab was used from this database, with subsequent removal of safety factors to provide either NOEC, LOEC or LC50 values. Once this value was identified, the Panel included its own 10x uncertainty/safety factors to estimate chronic toxicity. An additional 10x factor was assessed if the compound was determined to have significant endocrine disrupting potential based on U.S. EPA Comptox allocation or evidence in the scientific peer-reviewed literature. Lastly, another 10x factor was used to estimate saltwater toxicity from freshwater toxicity data.

- No toxicity values available from these three databases – the peer-reviewed literature was used to develop a threshold value and subsequent safety factors applied as described above.

- Sediment MTLs – The Panel did not address sediment as a matrix in this report. However, a similar approach would be used, as described above for the freshwater aqueous derivation. Essentially, chronic NOECs would be targeted, and if not available, a 10-fold safety factor would be implemented for acute:chronic uncertainties. A 10-fold safety factor for EDC potential would be used if the compound is identified as such by the U.S. EPA CompTox database, and a 10-fold safety factor would be included when deriving for estuarine/marine MTLs if toxicity values are unavailable for organisms in these media.
- Updating MTLs - The MTLs used were based on literature, with new data and values published over time. Accordingly, the Panel recommends periodic updating of MTLs to reflect new knowledge.

### 7.1.3 CEC Dashboard Visualization

The State Water Board intends the collected CEC data to be useful, accessible, and interoperable; inform all water stakeholders about water quality in water bodies of interest; and fundamentally support the mission of the State Water Board CEC Program. Consistent with the goal to enhance its data culture, the State Water Board invested in a data tool kit to support the State Water Board staff to access, manipulate, analyze, and interactively visualize data. For the purpose of the Panel efforts, *Tableau* (Tableau Software, LLC) was selected as the initial platform that provides a simple interface for interactive geospatial evaluation and allows for advanced data analysis on large or multiple datasets with simple interfaces and dashboards.

### 7.1.4 Updated Risk-Based Screening Approach

As previously noted, the updated risk-based screening approach of the Expert Panel as a "proof of concept" provides three features: an initial prioritization of CEC compounds of interest ('preliminary monitoring screening'), an approach to further narrow with priorities based on data availability, data quality, and spatial and temporal analyses ('refined monitoring screening'), and additional programmatic recommendations for the State Water Board staff to move forward (e.g., refinement of MDLs or MTLs or both). The screening process has been updated to prioritize CECs for monitoring based on a combination of the magnitude of the MTQ and the presence or absence of a trend in concentration (Figure 7.2). Thus, the overall CEC identification and prioritization process is divided into two screening stages.

1. **Preliminary Monitoring Screening** – consists of a conservative preliminary monitoring prioritization screening based on available data and MTLs that are used to calculate an $MTQ_{detect,}$, $MTQ_{sub}$ and trend. The preliminary monitoring prioritization categorizes CECs as either needing to be retained for possible inclusion in a monitoring program or eliminated from consideration in a current

monitoring program. CECs that are eliminated from consideration in a monitoring program based on current data can be evaluated again using the preliminary monitoring prioritization screening process if additional data are collected or if MTLs change. CECs that are retained for possible inclusion in a monitoring program are categorized as having either 'High', 'Moderate' or 'Low' monitoring priority.

2. **Refined Monitoring Screening** – this screening stage refines the monitoring prioritization by taking into account sample size, differences between $MTQ_{detect}$ and $MTQ_{sub}$, geographic and temporal distribution of monitoring data to evaluate the presence of trend, and comparison of MDLs to MTLs. The refined monitoring prioritization framework consists of a table (Figure 6.2.1) and 10 decision tree diagrams. The first decision tree diagram is referred to as the Initial Decision Tree (Figure 6.2.1). Each of the 10 decision tree diagrams (Appendix G, Figures G.1 through G.10) correspond to one of the 10 preliminary monitoring prioritization outcomes.

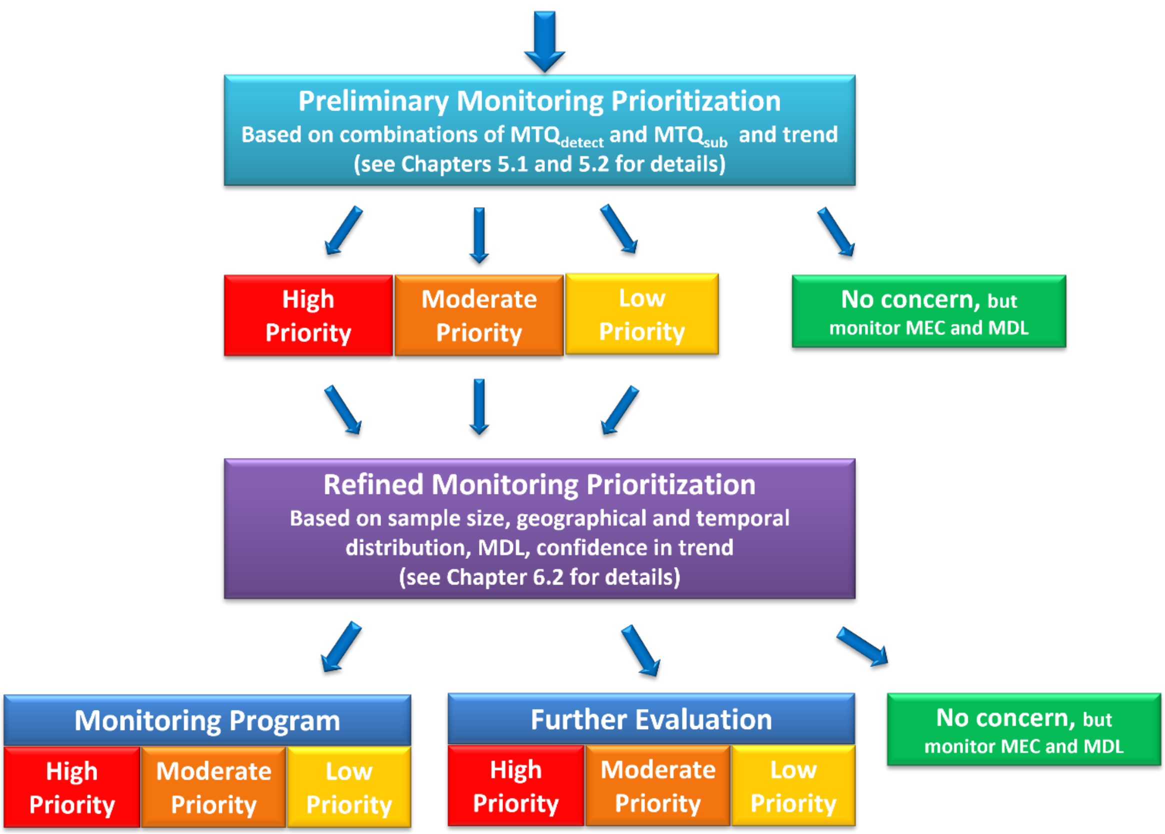


**Figure 7.1 Selection framework for constituents of emerging concern (CECs) using the State Water Board dataset.**

Table 7.2 presents a summary of the outcome of the initial prioritization for fresh, estuarine, and marine waters. In all three media about a fifth to a third of CECs were categorized as 'High' priority, between a third and a half were not a monitoring priority (out) and the remainder were categorized as either 'Moderate' or 'Low' priority. Almost all CECs categorized as 'Moderate' priority had $MTQ \leq 1$ (the exceptions are atenolol, bensulide, diazepam and warfarin in freshwater which have MTQ between 1 and 10) indicating the categorization is based on evidence of an increasing trend in concentration. In both fresh and marine waters about a third of the categorizations are based on $MTQ_{detect}$ and the remainder on $MTQ_{sub}$. In estuarine waters about 60% of the categorizations are based on $MTQ_{detect}$ and the remainder on $MTQ_{sub}$. Regardless of the media, when $MTQ_{sub}$ is used for the prioritization, $MEC_{sub}$ is equal to the median MDL. In other words, the assumed concentration of non-detects is driving the prioritization. When $MTQ_{sub}$ is used for the prioritization, almost all CECs categorized as 'High' have a median MDL>MTL and all CECs categorized as not a monitoring priority ('Out') have have median MDL<MTL demonstrating the importance of the combined effect of elevated MDLs with conservative MTLs on the initial prioritization process. It is possible that with lower MDLs or refined MTLs the priority of several of, perhaps even many of, the CECs currently categorized as 'High' based on $MTQ_{sub}$ would decrease.

To evaluate the effect of the refined prioritization step as a proof of concept, the refined prioritization was applied to eight CECs (five freshwater, two marine water, and one estuarine water). Six of the CECs had an initial prioritization of 'High'. After application of the refined prioritization portion of the framework, four remained a 'High' priority and two were identified as needing additional study. Both CECs with an initial 'Moderate' prioritization were identified as needing special study. The proof-of-concept application of the refined portion of the prioritization framework indicates such application is workable, will refine prioritization of CECs for monitoring and will help identify data gaps that need to be addressed to determine a CEC's monitoring priority, but it also suggests even after application of the refined prioritization a large number of CECs will remain a high monitoring priority.

The intent is for the State Water Board CEC Program staff to continue to implement the Panel's "proof of concept" by adopting the CEC risk-based prioritization and following through on broader implementation such as to improve the quality of CEC data reported to the State Water Board, update data systems, update MTLs as new CEC monitoring and toxicology information become available and document any potential modifications to the approach. The State Water Board CEC Program staff would then work with a future CEC Advisory Panel (or similar process) that would review the State Water Boards staff's implementation of their risk-based prioritization approach and other CEC Program activities, to provide feedback and additional recommendations that could ultimately be used to inform the State Water Board CEC Program and a CEC monitoring program.

The two-stage risk-based screening framework is not uniquely applicable to the State Water Board CEC dataset. If other datasets have available monitoring data, the screening and prioritization process can be applied to those as well.

**Table 7.2 Outcome of applying the preliminary monitoring prioritization to different matrices, including the total number (N) of constituents of emerging concern (CECs) within each category, their monitoring trigger levels (MTQs) for both detected values ($MTQ_{det}$) and substituted values ($MTQ_{sub}$), and the number and percentage for which their method detection limits (MDLs) or measured environmental concentrations (MECs) compared with their monitoring trigger levels (MTLs).**

| Freshwater (294 CECs total) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Metric | Preliminary Monitoring Priority (N) | Preliminary Monitoring Priority (% of total) | $MTQ_{det}$ (N) | $MTQ_{det}$ (% of total) | $MTQ_{sub}$ (N) | $MTQ_{sub}$ (% of total) | $MTQ_{sub}$ and MDL>MTL (N) | $MTQ_{sub}$ and MDL>MTL (%$MTQ_{sub}$) | $MTQ_{sub}$ and MEC=MDL (N) | $MTQ_{sub}$ and MEC=MDL (%$MTQ_{sub}$) |
| High Priority | 105 | 36% | 13 | 4% | 92 | 31% | 86 | 93% | 92 | 100% |
| Moderate Priority | 30 | 10% | 13 | 4% | 17 | 6% | 4 | 24% | 17 | 100% |
| Low Priority | 56 | 19% | 13 | 4% | 43 | 16% | 32 | 74% | 43 | 100% |
| Out Priority | 103 | 35% | 43 | 15% | 60 | 20% | 0 | 0% | 60 | 100% |

| Estuarine (276 CECs total) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Metric | Preliminary Monitoring Priority (N) | Preliminary Monitoring Priority (% of total) | $MTQ_{det}$ (N) | $MTQ_{det}$ (% of total) | $MTQ_{sub}$ (N) | $MTQ_{sub}$ (% of total) | $MTQ_{sub}$ and MDL>MTL (N) | $MTQ_{sub}$ and MDL>MTL (%$MTQ_{sub}$) | $MTQ_{sub}$ and MEC=MDL (N) | $MTQ_{sub}$ and MEC=MDL (%$MTQ_{sub}$) |
| High Priority | 51 | 18% | 26 | 9% | 25 | 9% | 23 | 96% | 25 | 100% |
| Moderate Priority | 17 | 6% | 11 | 4% | 6 | 2% | 1 | 17% | 6 | 100% |
| Low Priority | 48 | 17% | 28 | 10% | 20 | 7% | 5 | 20% | 20 | 100% |
| Out Priority | 161 | 58% | 99 | 36% | 63 | 22% | 0 | 0% | 63 | 100% |

| Marine (75 CECs total) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Metric | Preliminary Monitoring Priority (N) | Preliminary Monitoring Priority (% of total) | $MTQ_{det}$ (N) | $MTQ_{det}$ (% of total) | $MTQ_{sub}$ (N) | $MTQ_{sub}$ (% of total) | $MTQ_{sub}$ and MDL>MTL (N) | $MTQ_{sub}$ and MDL>MTL (% $MTQ_{sub}$) | $MTQ_{sub}$ and MEC=MDL (N) | $MTQ_{sub}$ and MEC=MDL (% $MTQ_{sub}$) |
| High Priority | 26 | 35% | 12 | 16% | 14 | 19% | 14 | 100% | 14 | 100% |
| Moderate Priority | 0 | 0% | 0 | 0% | 0 | 0% | NA | NA | NA | NA |
| Low Priority | 19 | 25% | 6 | 8% | 13 | 17% | 7 | 54% | 13 | 100% |
| Out Priority | 30 | 40% | 9 | 12% | 21 | 28% | 0 | 0% | 21 | 100% |

As was the case with the CEC screening process developed in 2012, categorizing a CEC as ‘High’ monitoring priority does not mean the CEC poses a potential risk, but rather warrants further investigation. Several conservative assumptions were used to establish the MEC and the MTL. Ibuprofen in freshwater is an example of a CEC where the initial categorization as a high monitoring priority in freshwater (A1, see Table Appendix Freshwater High Priority) likely greatly overstates monitoring priority and potential risk. The initial categorization is based on an $MTQ_{sub}$ of 1,000. However, the initial categorization does not take into account that ibuprofen was not detected in any of the 335 samples collected statewide and that the MTL is 1,000 times lower than median detection limit (see Appendix J, Table J.1). Thus, even though ibuprofen has one of the higher freshwater MTQs, because it is not detected and the detection limit is three orders of magnitude above the MTL, the MTQ of 1,000 is not indicative of a high potential risk.

The Panel cannot stress strongly enough that the MTQs generated as part of the prioritization process described above cannot and should not be interpreted as representing estimates of potential risk. As was the case with the CEC screening process developed in 2012, categorizing a CEC as ‘High’ monitoring priority (or “Moderate” or “Low” priority) based on its MTQ does not mean the CEC poses a potential risk, but rather only that the CEC warrants further investigation. Several conservative assumptions were used to establish the MEC and the MTL. Two CECs with some of the highest MTQs estimated using the above process exemplify the need to review the basis of all CECs with MTQs greater than unity.

Caffeine has one of the five highest $MTQ_{sub}$ values in freshwater (100,000) driven by the median MDL, as well as a high freshwater $MTQ_{detect}$ of 11,000. In estuarine waters the $MTQ_{detect}$ and $MTQ_{sub}$ are 570,000 and 360,000, respectively, and are the highest of all CECs. The Panel recognizes these MTQs cannot represent an estimate of possible effects in fresh or estuarine waters. Rather, the magnitude of the MTQs is a clear indication that closer examination of the basis for the MTQs is necessary. In the case of caffeine, that closer examination begins with the MTL of 0.0001 ug/L in freshwater and 0.00001 ug/L in estuarine water. The MTQs are based on detected concentrations and sample size, and both are sufficient such that their use to estimate the $MTQ_{detect}$ does not appear to be a limitation. This value is based on 551 detects in freshwater and 14 detects in estuarine waters. The MTLs are orders of magnitude below commonly achievable analytical detection limits and, therefore, almost certainly were not based on analytically measured concentrations in the toxicity studies. Closer review of the MTL reveals that it is based on a PhD dissertation from the USEPA CompTox database and utilized nominal concentrations only. Consequently, upon subsequent evaluation, use of nominal concentrations would flag this as a poor study and a re-evaluation of the toxicity threshold should be performed. In the case of caffeine, CompTox has chronic values that can be used, and the doses used for the EDC determination are not environmentally relevant. Consequently, the safety factors should not be applied and using the chronic toxicity value results in a refined MTL in the mg/l range. The corresponding MTQs are substantially less than unity, indicating that caffeine is not a monitoring priority in either fresh or estuarine waters. The Panel emphasizes that toxicity values e.g., MTLs that are substantially below the MDL (e.g., 5-fold or more) should be regarded with caution, and may warrant additional consideration in prioritization.

Ibuprofen in freshwater is another example of a CEC where the initial categorization as a “High” monitoring priority in freshwater (A1, see Table Appendix Freshwater High Priority) likely greatly overstates monitoring priority and cannot and should not be used as an indicator of potential risk. The initial categorization is based on an $MTQ_{sub}$ of 1,000. However, the initial categorization does not take into account that ibuprofen was not detected in any of the 335 samples collected statewide and that the MTL is 1,000 times lower than median detection limit (Appendix H, Table H.1). Thus, even though ibuprofen has one of the higher freshwater MTQs, because it is not detected and the detection limit is three orders of magnitude above the MTL, the MTQ of 1,000 is not indicative of a high monitoring priority or of the presence of a potential risk. As with caffeine, the basis for the MTL of 0.01 ug/L could be reviewed. However, the representativeness of the median MDL of 10 ug/L in the dissolved matrix should likely be reviewed first and perhaps set aside as ibuprofen in the total matrix has a median MDL of 0.02 ug/L and a corresponding $MTQ_{sub}$ of 2; 500 times lower than the more conservative MTQ used by the prioritization process based on the dissolved matrix MDL.

Both caffeine and ibuprofen speak directly to the aforementioned emphasis by the Panel that MTQs are not indicators of potential risk. Rather, that based on the above intentionally conservative monitoring process, the State can be confident that MTQs of less than one (1) indicate a CEC is not a monitoring priority and that MTQs of greater than unity indicate the need for review of the assumptions used to derive the MTL and MEC to confirm they are representative. It is only after such review that an appropriate MTQ can be derived, and the monitoring priority of a CEC established. Review of such re-evaluations of MTLs is a possible charge for a subsequent Expert Panel.

Recognizing the cautions, the Panel felt use of conservative assumptions was appropriate for determining whether a CEC should be included in a monitoring program. Such conservative assumptions need to be refined prior to determining the monitoring priority of a CEC and especially whether a potential risk may be present. That is a key reason the Panel included a second more refined step in the prioritization methodology. One of the outcomes of that second step is the identification of some possible additional considerations to better understand and refine the monitoring priority. Some such additional considerations are discussed for some of the example CECs in Chapter 6.2.

## 7.2 Future Maintenance of Dataset and Dashboard

The CEC dataset is currently housed as a static file of CEC occurrence data from statewide databases of environmental occurrence data (updated ASC Report) and voluntary CEC monitoring data compiled from MS Excel™ submittals provided to State Water Board following an email request to publicly owned treatment works (POTWs) in California. The existing State Water Board dataset is for a specific list of CEC classes and analytes (see Appendix J) and was developed with specific data boundaries with a focus on samples collected since 2005 to the present from ambient ecosystems (all matrices including water, sediment, biota, etc.) and relevant sources (e.g., wastewater, stormwater, recycled water, etc.).

Moving forward, the CEC dataset should be further updated to collect the most current CEC occurrence data directly from statewide databases using similar methods and procedures similar to those used by the ASC Data Synthesis Project, with the ability to incorporate voluntary data submittals provided by various POTWs, stakeholders, and/or research projects within the State. It is the Panel's understanding that the data update process will be documented in a forthcoming CEC Program Data Management Plan that will include development of a data dictionary and associated metadata. The CEC Program Data Management Plan should be written with a goal to publish the dataset following California's Open Data Portal guidelines (see Open Data Publisher Guide Contents – California Open Data). The approach should also include development of an automated process that queries available databases (including CEDEN, Water Quality Portal, SDWIS, CIWQS, and Geotracker) for updated CEC data submittals. CEC data should then be saved with appropriate metadata to document the details about the source of the data and provide appropriate citation to the original database. CEC occurrence data should subsequently be curated using the data curation steps developed with the Panel input (described in Chapter 5). In addition, the State Water Board data submittal portals (see sources of data previously described) need to incorporate specific quality assurance protocols (i.e., automated checking that rejects out of specification entries) for data input as described in Chapter 3. Finally, the Panel anticipates that the data acquisition and curation should evolve over time to incorporate additional CEC classes and analytes, as appropriate, and to enhance or develop additional data fields to streamline downstream data analyses.

The State Water Board data submittal portals (see sources of data previously described) need to incorporate specific quality assurance protocols (i.e., automated checking that rejects out of specification entries) for data input as described in Chapter

3. The following is a brief summary of operating procedures to improve Quality Assurance that should be developed by the State Water Board CEC Program in collaboration with the Office of Information, Management and Analysis and the State Water Board's Quality Assurance Officer to improve data quality, analysis and public access.

## Recommendations for Updating the CEC Dataset and Dashboard

- Encourage the use and acceptance of data from performance-based analytical methods with documented QA/QC procedures to expand the analytical capacity for monitoring CECs, especially "new" CECs, while ensuring data quality. Such methods can be non-commercial research methods;

- Establish strict QA/QC for data entries in the future; provide list of minimum entry parameters; automate QA/QC at point of data entry and submission;

- Periodically transfer and review the quality of CEC data from the various Water Board data portals (CIWQS, CEDEN et al. see Chapter 2);

- Establish rules for data entry. Two key examples based on the Panel's review of the existing dataset:

    - For a record to be valid, all fields must have an entry (e.g., latitude and longitude for the sample),

    - For some fields, the Panel recommends developing valid values (e.g., MDLs);

- Review literature (published as well as grey literature) to inform Water Board staff regarding potential new emerging CECs; consider persistent, mobile, and bioaccumulative chemicals;

- Periodically update Dashboard with QA dataset. At a minimum, the CEC dataset should be published and made accessible to the public through an open data format. This approach should be coordinated through the Office of Information Management and Analysis and should establish public access to the CEC dataset with the potential to support data visualization and interpretation using programs such as Tableau, PowerBI, and/or ArcGIS. A link to the published dataset should be provided through the CEC Program website, including the version of the database to indicate when the dataset has been updated.

### Recommendations for Updating Risk-Based Screening Information

- Review toxicity literature and databases to update and refine MTLs;
- Continue compiling MTLs for marine water, sediments, tissues;
- Periodically update risk-based screening results based on updated occurrence dataset and updated MTLs.

### Recommendations for Developing Implementation Process and Procedures

- Develop a process for how and when to handover certain CECs/CEC classes to other Water Board or state agency programs for evaluation beyond monitoring. For example, a CEC with many years of data and MTQs consistently greater than 10 might be a candidate for refinement of its MTL, or special studies to verify whether adverse effects are occurring in ambient waters, or development of ambient water quality criteria, among others.;
- Further define Risk-Based Screening Monitoring endpoint recommendations – monitoring recommendations (see discussion in Chapter 7.3);
- Establish a process for an external panel or scientific review process (see Chapter 7.4) to review regularly:
    - Standard Operating Procedures and QA/QC of the dataset,
    - updated toxicity endpoints and MTLs,
    - results of literature review,
    - updated Risk-Based screening results (includes status and results of implementing operating procedures noted above), and results of new data collected as part of special monitoring studies, which may include bioassays and NTA.

## 7.3 Additional Considerations and Recommendations

This Panel spent substantial amounts of thought and time refining and updating the risk-based CEC monitoring approach presented in our earlier report (Anderson et al. 2012). Updating the monitoring prioritization screening methods has allowed the Panel to develop an appreciation for their intricacy and realize that they are one aspect of refining the CEC-by-CEC and CEC class-based monitoring approach. The others (e.g., organizing the MEC data and dataset, QA of the data and analytical methods, reviewing toxicity data and deriving MTLs, developing recommended monitoring programs, etc.) are also complex and time consuming. This has led the Panel to wonder whether expecting the State Water Board CEC Program staff to successfully implement the commonly used CEC-by-CEC ("reductionist") approach is realistic? If a key goal is to avoid a 'new surprise' (e.g., perchlorate, PFAS, antioxidant and antiozonant compounds in tire leachate), the Panel is concerned that several reasons exist to believe that key goal will not be achieved if the State continues to monitor for CECs using exclusively a CEC-by-CEC reductionist approach. Additionally, the Panel would like to point out that only a few instances exist where a CEC-by CEC monitoring approach has predicted an adverse effect from a CEC before the effect was observed in ambient waters.

First, is it reasonable to expect that the State Water Board CEC Program staff will be able to recommend analytical methods with specified MDLs and reporting limits for existing and newly added CECs, have those uniformly adopted by the entities that are performing the monitoring, have the collected information correctly entered into the database (more or less), and then have State Water Board CEC Program staff QA those data such that the State Water Board and future Panels have a high degree of confidence in the representativeness and usability of those data? Based on the current Panel's experience over the past nearly two years, that does not seem a reasonable series of assumptions. That is not a reflection of the State Water Board CEC Program staff. Rather, it reflects the many pronged nature and complexity of the process used to collect and summarize CEC data and the practical limitations experienced by State Water Board CEC Program staff to exert the necessary level of control and oversight of all of those steps given the current resource allocations.

Second, even assuming robust and reliable MEC data can be collected and compiled, MTLs and the CEC monitoring prioritization process will need to be updated on a regular basis. Following such updates, either new monitoring programs will need to be developed and implemented or existing programs modified and refined. Such review and refinement are likely doable for 10-25 CECs, particularly if portions of the monitoring prioritization screening process are part of the Dashboard (at least the initial steps). However, keeping in mind that the latter stages of the CEC prioritization process require professional judgment on a CEC-by-CEC basis, conducting such refinement for 200 or more CECs as the list of candidate CECs grows seems a daunting task.

Third, and perhaps most importantly, even if the State Water Board CEC Program staff are able to accomplish both of the above, is the CEC-by-CEC process going to identify the "next major actor" or even locations where effects from known actors are occurring and which of the known actors are responsible for those effects? Likely not. Would a CEC-by-CEC monitoring program of the type used to date have identified the antioxidant and antiozonant compounds tire leachate affecting salmon? PFAS? Even hormones? Absent information from other programs and settings that lead to the identification of possible new individual or classes of CECs suspected of causing an effect, that new CEC would not even be on the list.  Similarly, the effect of compounds present in aquatic systems but that do not have toxicity information to develop MTLs also cannot be evaluated to determine if they should be on a monitoring list. The CEC monitoring list is analogous to the often used example of looking for keys at night under a lamppost because that is the only area that is lit. This speaks directly to this Panel's recommendation that the CEC list be updated and expanded based on review of non-California sources for new classes of CECs (see Chapter 3). Though even those new CECs may have been found only because different groups of investigators in other geographic locations were looking under different lampposts, but lampposts still. This raises the question of how one looks into the dark beyond the lit area under lampposts?

Use of a class-based or chemical grouping approach, that identifies individual compounds based on similar chemical structure as well as by function or use, could certainly widen the lit area under the lamppost. The approach was adopted in the ASC report (Sutton et al 2022) and is broadly applied in chemical risk assessment of industrial chemicals (OECD 2014). A class-based approached has been used for PFAS related chemicals by the State Water Board PFAS Action Plan (https://www.waterboards.ca.gov/pfas/) but it could be more widely applied to identify industrial chemicals of possible concern. Bisphenols, phthalates, alkyl phenols, and organophosphate ester flame retardants are examples of classes identified in the ASC report that could be expanded. Indeed, the ASC report included new classes (siloxanes, plastic monomers, additives, and processing aids, vehicle and tire-related contaminants, and quaternary ammonium compounds, in a list of potential new CECs. However, individual chemicals within all classes may have different modes of action and thus different toxicological profiles.

The Panel's previous Expert Report(s) (Anderson et al. 2012) suggested bioanalytical methods as an approach to screen for effects of contaminants in surface waters. Chapter 3 discussed the advantages of combining bioanalytical methods with NTA as two key elements when conducting effects-based analysis.  Based on the information available to this Panel, bioanalytical methods do not seem to have been widely implemented even though many are standardized and widely available for some key endpoints. They remain a monitoring methodology the Panel recommends be used regularly and widely.  Such methods are especially critical for human health, as monitoring human populations for adverse effects is unlikely to be part of a recommended monitoring plan or that limits are adequately protective of aquatic life and water quality).  Likewise, agencies have invested in expensive and complex high-resolution mass spectrometers necessary for instrumental NTA with the intention of using them for CEC discovery.  However, instrumental NTA has limitations as discussed in Chapter 3, such as limited sensitivity due to its typically not being optimized to detect any specific set of compounds. The Panel recommends use of both bioanalytical methods to find effects, alongside instrumental NTA to search for compounds that may cause these effects, and targeted chemical analysis to quantify such compounds when appropriate standards exist.

Another more holistic monitoring method is long-term measurement of a range of in-stream biological endpoints. The pulp and paper industry implemented this approach in the past two decades in response to concerns about the menagerie of compounds in mill effluents (McLaughlin and Flinders 2016, Flinders et al. 2009a,b, Flinders et al. 2015). It was easier to actually look for effects in receiving waters than to try to analyze effluent for the menagerie and then develop the exposure and toxicity information necessary to conduct a risk assessment for all those individual compounds. The industry identified several mills covering a range of process types, geographies and streams (e.g., cold-water and warm-water; west and east) and monitored receiving waters both upstream and downstream of each mill for several years (Hall et al. 2009a,b).

California might be able to do the same by identifying the situations/settings with the greatest potential for CEC release (e.g., agricultural, POTW, urban runoff) and then establish long-term monitoring locations in various parts of the state (e.g., Central Valley, Southern California, Bay area, freshwater, estuarine water, marine water). Review of existing MTQs may already provide a sense of areas with greatest potential to observe an effect. Some form of a compiled MTQ (e.g., arithmetic mean of the CEC-specific MTQs within a geographic area/discharge point) could be used to identify geographic areas/receiving waters with the greatest potential to be adversely affected. No doubt this would take time and effort to plan and implement but it might be a better use of limited resources than trying to manage and expand the existing CEC-by-CEC monitoring program. Combining in-stream monitoring with effects-based analysis (i.e., NTA and bioanalytical methods) should also help link bioanalytical responses to real world effects. If links can be established, the bioanalytical responses could be used for monitoring rather than the in-stream measurements given the latter are likely substantially more resource intensive. If effects are found by either monitoring biological endpoints in receiving waters or bioanalytical methods, then the search can begin for the causative agent(s), which may or may not be CECs.

The Panel is not suggesting the existing CEC-by-CEC program be eliminated. It would continue at a baseline level. The existing program is important because it informs the State about current conditions and whether those are changing for CECs on the list. The current CEC-by-CEC monitoring approach does require known toxicity data (e.g., MTLs) before it can be recommended for monitoring, e.g., MECs above an MTL implies the potential for adverse effects to aquatic life. But it does not determine whether adverse effects are actually occurring. Nor does it inform the State whether an existing CEC could become an issue in the future, although the "trend analysis" included in the refined monitoring prioritization methodology described Chapters 5 and 6 is a step in that direction. A better way would be to have information about the changes in use of compounds in commerce with a focus on existing compounds whose use is increasing and new compounds entering the market. That information could be used to develop screening level PECs and determine whether those compounds should be added to the monitoring list.

## 7.4 Role of Expert Panels

The role of the future Expert Panel should be to provide advice on specific technical issues and not function as a Q&A discussion panel with experts. Thus, the Expert Panel should be formed as a standing State Water Board Panel and focus on providing review and advice in the following areas:

- monitoring program development and implementation;
- professional or scientific matters to supplement staff expertise;
- scientific advice where there is lack of conclusive data or scientific certainty.

- Charges – at a minimum the Expert Panel should provide technical/scientific review of the following items:
    - QA/QC SOP for data set updates;
    - Risk-Based Screening Monitoring endpoint recommendations (e.g., process/programs and recommendations to move beyond routine constituent monitoring and results of new data collected as part of special monitoring studies);
    - Updated MTLs;
    - Results of literature review;
    - Updated Risk-Based screening results.
- Review cycles – the future Expert Panel should meet at periodic intervals as appropriate, depending on mutual agreement between the Panelists and requisite State Water Board staff (e.g., CEC Program, among others). A suggested frequency would be twice per year.

# 8. Overarching Observations and Recommended Next Steps

The Panel's overarching observations and recommended next steps are presented in this Chapter.

The 2012 Expert Panel had developed a risk-based framework to prioritize CECs for monitoring. The fundamental approach of that framework was a risk-based comparison of MECs to MTLs. A central question for the 2022 Panel was to see if the same or similar risk-based approach remained applicable to the much larger current dataset. Given that one of the long-standing goals of the State's CEC monitoring program is to reduce CEC "surprises" in the future, the Panel expanded the original risk-based screening framework to account for trend in concentration, if available, along with information about MEC and MTL. Because the Panel intentionally selected a highly conservative preliminary prioritization step (i.e., one that uses the 90$^{th}$ percentile of either the $MEC_{detect}$ or $MEC_{sub}$, and MTLs based on the most conservative reproductive endpoint available from the literature or other sources), the Panel added a second step to the CEC prioritization framework to refine some of the highly conservative assumption in the initial prioritization. The refined prioritization gave greater weight to detected concentrations than non-detects (i.e., $MEC_{detect}$ than $MEC_{sub}$), took into account sample size, and reviewed the basis for trends. As with the initial prioritization step of the framework, the outcome of the refined monitoring prioritization is a conservative prioritization of CECs. It is not an assessment of potential risk and MTQs of greater than unity do not indicate that adverse effects are present. They only indicate that a CEC may need to be included in a monitoring program.

The State and its contractors have been compiling and reviewing data since 2005. As the Panel delved into the data, it identified numerous data quality issues. State Water Board CEC staff worked closely with the Panel for the past two years to improve the quality of the existing dataset and to develop tools to better visualize the volumes of data collected by the State. The CEC data visualization dashboard developed by State Water Board CEC staff represents a terrific advance that will enable stakeholders to better understand the breadth of sampling conducted. While many data quality issues were corrected, the quality of some aspects of the existing dataset (e.g., MDLs) remains a concern and affects the utility of the dataset.

Recognizing that the remaining dataset still had quality limitations, the Panel nevertheless applied the updated framework using the existing dataset as a 'proof of concept' to prioritize CECs for monitoring. When the preliminary prioritization step of the expanded framework was applied to the current dataset, 186, 152 and 48 CECs were classified as a monitoring priority (either high, moderate or low priority) in fresh, estuarine and marine waters, respectively. That compares to a total of 9, 7 and no CECs identified for monitoring in fresh, estuarine and marine waters, respectively, by the 2012 Panel. Application of the refined prioritization step of the framework to eight example CECs suggests it will help identify data gaps that need to be addressed to determine a CEC's monitoring priority and may reduce the number of CECs requiring monitoring, but it also suggests a much larger number of CECs will be a monitoring priority than identified by the 2012 Panel.

While reviewing the outcome of the updated prioritization framework, the Panel realized that many CECs have MTLs that are less than their respective MDL. That leads to a CEC being a monitoring priority (either high, moderate or low depending upon magnitude of MTQ and trend based on the initial prioritization step) even though the CEC may not have been detected or was detected very infrequently. For some CECs the MTQ may exceed 1 because the MDL is elevated. In such cases the value of such data points (records) should be further evaluated before being used to reach a conclusion about monitoring priority. For other CECs, the MDL may represent the best that labs can accomplish and the MTL is simply lower. However, as described in Chapter 4, the MTLs identified in this report and used in the prioritization framework were intentionally selected to be conservative. For some CECs, they may be more conservative than necessary to protect aquatic life and ecosystems in California waters.

The Panel also used sources beyond the State Water Board dataset, both within the State of California and outside of it, to identify a total of 135 CECs not currently included in the State Water Board dataset but whose monitoring priority should be evaluated.

Based on the level of effort over the past 2+ years it has taken the Panel and State Water Board CEC staff to develop the updated risk-based monitoring prioritization framework and to apply to it a few CECs as a 'proof of concept', the Panel is acutely aware of the technical and resource challenges posed by developing monitoring programs on a CEC-by-CEC approach. When occurrence data were relatively limited and candidate CECs relatively few, as in 2012, the occurrence data compilation to establish MECs and toxicity literature review to derive MTLs was manageable. With the current list of CECs requiring evaluation and consideration for monitoring approaching 500, the resource and quality control challenges are immense and will continue to grow. The Panel has substantial concern as to whether focusing the State's limited resources and staff on the CEC-by-CEC approach represents the best way to assure California residents and stakeholders that the presence of CECs in ambient waters are not posing a risk to aquatic life and ecosystems.

Lastly, in the 10 years between the 2012 and 2022 Panels a great deal in the world of CECs has changed. In 2012 CEC monitoring was still in early stages with limited data, approaches, and monitoring programs. As a result, the 2012 Panel was able to summarize existing California-specific data to derive MECs, review toxicity data to develop MTLs and create a risk-based framework for CEC monitoring, among other efforts. In the intervening 10 years the CEC field has developed exponentially, and the State now has staff dedicated to monitoring and evaluating CECs. That requires a transition in the role of a Panel. Panels should no longer be expected to summarize data and develop approaches. That effort should be taken up by State staff and the results of that effort presented to a Panel for review and comment.

Key recommendations from the Panel's evaluation are:

1. Existing occurrence data need further refinement and quality assurance before they can be used to develop a final list of prioritized CECs. State staff need to develop methods and decision criteria to identify and be able to use occurrence data of high quality to prioritize CECs for monitoring. A key area of focus will be elevated MDLs and MDLs>MTLs and how to better understand the effect of MDL uncertainty on CEC prioritization.

2. **Data collected in the future need to be of consistently high quality to be accepted into the dataset.** Refine data entry steps to minimize missing information such as detection limits, sampling location etc. that hamper full use of the data.

3. Establish and implement a procedure to transfer and review the quality of CEC data from other sources such as CEDEN et al. (data should be collected and reviewed at least semi-annually).

4. For CECs with MTL less than an achievable MDL, the Panel recommends SWB CEC staff review the derivation of the MTL to determine if the inherently high level of conservatism in the MTLs presented in this report is necessary to protect aquatic life and ecosystems in California waters. Similarly, the Panel recommends that for CECs with MTL>MDL, SWB CEC staff consider whether MDLs required by the monitoring program need to be as low as achievable or simply low enough to achieve the MTL.

5. Establish a procedure to review literature (published as well as grey literature) to inform SWB staff regarding potential newly emerging CECs making sure to take into consideration persistence, mobility, and bioaccumulation potential.

6. SWB CEC staff should apply the updated prioritization framework to all CECs in the High, Moderate and Low preliminary monitoring priority categories (see Chapter 6.1) to develop a refined CEC prioritization list for monitoring. Before implementing new monitoring programs, the Panel recommends that all aspects

of such updated programs, and their bases, be reviewed by a subsequent Panel or similar process.

7. **Define a process to address how and when to handover certain CECs/CEC classes to other SWB programs.** Specifically, the SWB staff need to consider the situation that at some point sufficient monitoring has occurred and the “status” of a CEC or CEC class changes from a monitoring program to another actionable program.

8. Establish a process that encourages the use and acceptance of data from non-commercial (research) analytical methods and documented QA/QC procedures.

9. The Panel recommends SWB CEC continue to refine the Visualization Dashboard and the incorporation of the CEC prioritization framework in the dashboard enabling the State to automate many of the steps necessary identify and prioritize CECs for monitoring, as well as identify the areas in California where monitoring for CECs would be most beneficial.

10. The Panel recommends the State explore alternative monitoring approaches to identify CECs that may pose a risk aquatic life and aquatic ecosystems in California including bioanalytical methods, use of PECs for CECs without California-specific MEC data; NTA; and effects-based biomonitoring in a few key locations/ecosystems.

11. The Panel recommends the State employ Expert Panels or similar processes in the future to review draft CEC prioritization and monitoring programs and approaches developed by SWB CEC staff and its contractors; future Expert Panels or similar processes should not be expected to develop such programs and approaches.

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