

# **Anthropogenic Organic Compounds in Source Water of Select Community Water Systems in the United States, 2002–10**

Scientific Investigations Report 2014– 5139



# **Anthropogenic Organic Compounds in Source Water of Select Community Water Systems in the United States, 2002–10**

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## Foreword

The U.S. Geological Survey (USGS) is committed to providing the Nation with reliable scientific information that helps to enhance and protect the overall quality of life and that facilitates effective management of water, biological, energy, and mineral resources (<http://www.usgs.gov/>). Information on the Nation's water resources is critical to ensuring long-term availability of water that is safe for drinking and recreation and is suitable for industry, irrigation, and fish and wildlife. Population growth and increasing demands for water make the availability of that water, measured in terms of quantity and quality, even more essential to the long-term sustainability of our communities and ecosystems.

The USGS implemented the National Water-Quality Assessment (NAWQA) Program in 1991 to support national, regional, State, and local information needs and decisions related to water-quality management and policy (<http://water.usgs.gov/nawqa>). The NAWQA Program is designed to answer: What is the quality of our Nation's streams and groundwater? How are conditions changing over time? How do natural features and human activities affect the quality of streams and groundwater, and where are those effects most pronounced? By combining information on water chemistry, physical characteristics, stream habitat, and aquatic life, the NAWQA Program aims to provide science-based insights for current and emerging water issues and priorities. From 1991 to 2001, the NAWQA Program completed interdisciplinary assessments and established a baseline understanding of water-quality conditions in 51 of the Nation's river basins and aquifers, referred to as Study Units ([http://water.usgs.gov/nawqa/studies/study\\_units.html](http://water.usgs.gov/nawqa/studies/study_units.html)).

National and regional assessments are ongoing in the second decade (2002–2010) of the NAWQA Program as 42 of the 51 Study Units are selectively reassessed. These assessments extend the findings in the Study Units by determining water-quality status and trends at sites that have been consistently monitored for more than a decade, and filling critical gaps in characterizing the quality of surface water and groundwater. For example, increased emphasis has been placed on assessing the quality of source water and finished water associated with many of the Nation's largest community water systems. During the second decade, NAWQA is addressing five national priority topics that build an understanding of how natural features and human activities affect water quality, and establish links between sources of compounds, the transport of those compounds through the hydrologic system, and the potential effects of compounds on humans and aquatic ecosystems. Included are studies on the fate of agricultural chemicals, effects of urbanization on stream ecosystems, bioaccumulation of mercury in stream ecosystems, effects of nutrient enrichment on aquatic ecosystems, and transport of compounds to public-supply wells. In addition, national syntheses of information on pesticides, volatile organic compounds (VOCs), nutrients, trace elements, and aquatic ecology are continuing.

The USGS aims to disseminate credible, timely, and relevant science information to address practical and effective water-resource management and strategies that protect and restore water quality. We hope this NAWQA publication will provide you with insights and information to meet your needs, and will foster increased citizen awareness and involvement in the protection and restoration of our Nation's waters.

The USGS recognizes that a national assessment by a single program cannot address all water-resource issues of interest. External coordination at all levels is critical for cost-effective management, regulation, and conservation of our Nation's water resources. The NAWQA Program, therefore, depends on advice and information from other agencies—Federal, State, regional, interstate, Tribal, and local—as well as nongovernmental organizations, industry, academia, and other stakeholder groups. Your assistance and suggestions are greatly appreciated.

William H. Werkheiser  
USGS Associate Director for Water

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## Conversion Factors

SI to Inch/Pound

<b>Multiply</b>	<b>By</b>	<b>To obtain</b>
	Length	
meter (m)	3.281	foot (ft)
kilometer (km)	0.6214	mile (mi)
	Area	
square kilometer (km <sup>2</sup> )	0.3861	square mile (mi <sup>2</sup> )
	Volume	
liter (L)	0.2642	gallon (gal)
	Flow rate	
liter per second (L/s)	15.85	gallon per minute (gal/min)

Vertical coordinate information is references to the North American Vertical Datum of 1988 (NAVD 88).

Horizontal coordinate information is referenced to the North American Datum of 1983 (NAD 83).

Concentrations of chemical constituents in water are given in micrograms per liter ( $\mu\text{g/L}$ ).

## Abbreviations and Symbols

<	less than
C<	censored concentration
µg/L	micrograms per liter
AHTN	acetyl hexamethyl tetrahydronaphthalene
AOC	anthropogenic organic compound
BQ	benchmark quotient
CCL	Contaminant Candidate List (U.S. Environmental Protection Agency)
CCL3	Contaminant Candidate List 3 (U.S. Environmental Protection Agency)
CWS	community water system
DEET	<i>N,N</i> -diethyl- <i>meta</i> -toluamide
E	estimated
EPA	U.S. Environmental Protection Agency
ESA	ethane sulfonic acid
GC/MS	gas chromatography/mass spectrometry
GRAS	Generally Recognized As Safe (U.S. Food and Drug Administration)
HBSL	Health-Based Screening Level (U.S. Geological Survey)
HHCB	hexahydrohexamethylcyclopentabenzopyran
HPLC/MS	high-performance liquid chromatography/mass spectrometry
LRL	laboratory reporting level
MCL	Maximum Contaminant Level (U.S. Environmental Protection Agency)
MEK	methyl ethyl ketone
MTBE	methyl <i>tert</i> -butyl ether
NAWQA	National Water-Quality Assessment (U.S. Geological Survey)
NWIS	National Water Information System (U.S. Geological Survey)
NWQL	National Water Quality Laboratory (U.S. Geological Survey)
PAH	polynuclear aromatic hydrocarbon
PCE	perchloroethene
PSDB	Public Supply Database (U.S. Environmental Protection Agency)
<i>p</i> -value	probability value
PVC	polyvinyl chloride
PWS	public drinking-water system
SDWA	Safe Drinking Water Act
SDWIS	Safe Drinking Water Information System (U.S. Environmental Protection Agency)

SWQA	Source Water-Quality Assessment (U.S. Geological Survey)
TCE	trichloroethene
UCMR	Unregulated Compound Monitoring Rule (U.S. Environmental Protection Agency)
USGS	U.S. Geological Survey
VOC	volatile organic compound

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## Abstract

Drinking water delivered by community water systems (CWSs) comes from one or both of two sources: surface water and groundwater. Source water is raw, untreated water used by CWSs and is usually treated before distribution to consumers. Beginning in 2002, the U.S. Geological Survey's (USGS) National Water-Quality Assessment Program initiated Source Water-Quality Assessments (SWQAs) at select CWSs across the United States, primarily to characterize the occurrence of a large number of anthropogenic organic compounds that are predominantly unregulated by the U.S. Environmental Protection Agency.

Source-water samples from CWSs were collected during 2002–10 from 20 surface-water sites (river intakes) and during 2002–09 from 448 groundwater sites (supply wells). River intakes were sampled approximately 16 times during a 1-year sampling period, and supply wells were sampled once. Samples were monitored for 265 anthropogenic organic compounds. An additional 3 herbicides and 16 herbicide degradates were monitored in samples collected from 8 river intakes and 118 supply wells in areas where these compounds likely have been used. Thirty-seven compounds have an established U.S. Environmental Protection Agency (EPA) Maximum Contaminant Level (MCL) for drinking water, 123 have USGS Health-Based Screening Levels (HBSLs), and 29 are included on the EPA Contaminant Candidate List 3. All compounds detected in source water were evaluated both with and without an assessment level and were grouped into 13 categories (hereafter termed as “use groups”) based on their primary use or source.

The CWS sites were characterized in a national context using an extract of the EPA Safe Drinking Water Information System to develop spatially derived and system-specific ancillary data. Community water system information is contained in the EPA Public Supply Database, which includes 2,016 active river intakes and 112,099 active supply wells. Ancillary variables including population served, watershed size, land use, population density, and recharge were characterized for

each of the watersheds for river intakes and contributing areas for supply wells.

A total of 313 samples were collected from 20 river intakes. Between the years of 2002 through 2010, samples were collected approximately 16 times over the course of a year. Seventy-one compounds from 12 of the 13 use groups commonly occurred (detected in greater than or equal to 1 percent of samples using an assessment level of 0.05 microgram per liter or when a compound was detected in greater than or equal to 10 percent of samples without an assessment level) indicating a wide variety of sources and pathways to these rivers and highlighting the importance of source-water protection strategies.

A total of 448 supply wells were sampled once during 2002–10 as part of 30 independent groundwater studies. About 15 CWS supply wells were sampled for each independent groundwater study. Twenty-eight compounds from 7 of the 13 use groups commonly occurred indicating a wide variety of sources and pathways exist for these compounds to reach these wells and highlighting the importance of wellhead protection strategies.

About one-half the 265 compounds monitored (122) were detected in both surface water and groundwater samples. A more diverse suite of compounds were detected in surface water in comparison to groundwater. However, herbicides and herbicide degradates were the most frequent group of compounds detected in both surface water and groundwater. Sixty-five of the most commonly occurring compounds were detected in one or more samples from both surface water and groundwater.

Human-health benchmarks (MCLs for regulated compounds and HBSLs for unregulated compounds) were available for more than one-half the compounds (160 of the 265) monitored in this study. Fifty-eight percent (41 of 71) of the commonly occurring compounds in surface water have a human-health benchmark to which concentrations can be compared; 19 have MCLs and 22 have HBSLs. Eighty-three percent (24 of 28) of the most commonly occurring compounds in groundwater have a human-health benchmark for

which concentrations can be compared; 14 have MCLs and 10 have HBSLs.

To put results from this study into context with the national distribution of river intakes and supply wells used by CWSs, sites were grouped into the respective national population of land-use quartiles. The increase in compound occurrence with increasing urban and agricultural land use in the watershed or contributing area was more evident for rivers than for supply wells. The increase in detection frequency of herbicides and herbicide degradates with increasing agricultural land use was more evident for rivers than for supply wells. The occurrence of solvents did not change substantially with increasing urban land use for rivers or supply wells.

Basic co-occurrence analyses were completed with and without an assessment level. Considering all detections in surface water without an assessment level, approximately 86 percent of source-water samples contained 2 or more compounds, and 50 percent of samples contained at least 14 compounds. Considering all detections in groundwater without an assessment level, 50 percent of samples contained at least three compounds. For the most part, the compounds detected most frequently as individual compounds in the environment often composed the most frequent unique mixtures. Five of the 10 most frequently co-occurring unique mixtures in both surface water and groundwater were the same: atrazine and deethylatrazine; atrazine and chloroform; deethylatrazine and simazine; atrazine and simazine; and deethylatrazine, atrazine, and simazine. Because similar mixtures were identified in both surface water and groundwater without an assessment level, future studies could be directed toward better understanding the toxicological importance of these unique mixtures.

Summed concentrations of herbicide degradates were compared to concentrations of the parent herbicides in surface-water and groundwater samples collected from 8 river intakes and 118 CWS wells, from which samples were analyzed for an additional 3 herbicides and 16 degradates. The toxicity to humans for many of these degradate products is largely unknown and thus points to the importance of monitoring these compounds (both the parent and degradate) in the environment.

This study highlights the importance of anthropogenic organic compounds in source water of select CWSs in the United States by characterizing their occurrence in surface-water and groundwater samples. Compound concentrations and occurrence are summarized and evaluated in a human-health context, when possible. Additionally, compounds found to co-occur as mixtures for both surface water and groundwater highlight the significance of low-level compound co-occurrence.

## Introduction

The quality of the Nation's drinking-water supply is an issue of national importance because it is essential to public

health (U.S. General Accounting Office, 1997). In 2008, about 155,000 public drinking-water systems (PWSs) were in operation in the United States (U.S. Environmental Protection Agency, 2010). A PWS is defined by the Safe Drinking Water Act (SDWA) as one that serves piped drinking water to at least 25 people or 15 service connections for at least 60 days a year (U.S. Environmental Protection Agency, 2003). Public drinking-water systems provide drinking water to about 312 million people. Only about 52,000 of the 155,000 PWSs are considered community water systems (CWSs) that supply water to the same population year round (U.S. Environmental Protection Agency, 2010). However, most of the population (about 292 million) receives their drinking water from CWSs (U.S. Environmental Protection Agency, 2003).

Drinking water delivered by CWSs comes from one or both of two sources: surface water and groundwater (hereafter termed "source water"). Source water is raw, untreated water used by CWSs and is usually treated before distribution to consumers. Finished water is defined as water that has passed through a water treatment plant, such that all the treatment processes are completed, or "finished" (Symons and others, 2000). Community water systems are required to monitor their finished water for about 90 regulated compounds; however, more than 22 million known organic and inorganic substances are known to exist, of which nearly 6 million are commercially available (Reiter and others, 2004; U.S. Environmental Protection Agency, 2009a). Current analytical capabilities cover only a very small fraction of compounds potentially in the environment that may enter our Nation's drinking-water supply (Olsen and others, 2013).

The SDWA was passed by Congress in 1974 to protect public health by regulating the Nation's public drinking-water supply (U.S. Environmental Protection Agency, 2009b). Originally, the SDWA aimed primarily at treatment as the means of providing safe drinking water. The SDWA was subsequently amended in 1986 and 1996; it now requires many additional actions, such as source-water protection, to protect source water and drinking water. The SDWA requires the U.S. Environmental Protection Agency (EPA) to establish enforceable national health-based standards, called Maximum Contaminant Levels (MCLs), for drinking water to protect against public health risks associated with naturally occurring and anthropogenic compounds (U.S. Environmental Protection Agency, 2004). The SDWA also broadly defines a "contaminant" as "any physical, chemical, biological, or radiological substance or matter in water" (U.S. Senate, 2002).

The SDWA gives the EPA the responsibility to periodically publish a list of unregulated compounds called the Contaminant Candidate List (CCL). The purpose of the CCL is to help assess the need for new drinking-water regulations to address occurrence of unregulated compounds. The most current list (as of 2013), Contaminant Candidate List 3 (CCL3), contains a list of 104 compounds or compound groups that currently are not subject to any proposed national primary drinking-water regulations, that are known or anticipated to occur in PWSs, and which may require regulation by the



SDWA in the future (U.S. Environmental Protection Agency, 2012a). After publishing each CCL, EPA also decides whether to regulate at least five compounds from the most current CCL in drinking water based on the compound's potential for adverse human-health effects, occurrence in PWSs, and a meaningful opportunity to protect public health; these decisions are called "regulatory determinations" (U.S. Environmental Protection Agency, 2012a). To help characterize the occurrence of compounds on the CCL3, the EPA required about 5,000 PWSs to monitor 25 of the compounds during 2008–10 as part of the Unregulated Compound Monitoring Rule (UCMR) (U.S. Environmental Protection Agency, 2008a). Data obtained from the UCMR on the occurrence of unregulated compounds, along with results from USGS and other monitoring activities, are used by EPA as part of both the CCL and regulatory determination processes (Toccalino and Hopple, 2010).

Unfortunately, sparse toxicity information exists for unregulated compounds to determine the significance of occurrence information in a human-health context. Furthermore, the occurrence of mixtures in source water is a matter of increasing concern and attention because the total combined toxicity of compounds in water may be greater than that of any individual compound. Little is known about the potential health effects associated with exposure to multiple compounds, and more investigation is needed to evaluate the potential toxicity of mixtures to humans (Hasegawa and others, 1994; Yang, 1994). In addition, little is known about the human-health significance of degradation products. For example, herbicide degradates may have less, similar, or greater toxicity than parent compounds (Hladik and others, 2005).

Characterizing source water is important to better understand, in part, which compounds occur through natural occurrence, animal activity, or as a result of anthropogenic effects. This information is valuable to regulatory agencies and water treatment industries. Additionally, the most frequently co-occurring compounds can be identified, which may guide future research to evaluate the potential toxicity of these mixtures to humans. Understanding co-occurrence of compounds is important because little is known on the cumulative human-health effects of multiple compounds that occur at low-level concentrations (Yang, 1994; Carpenter and others, 2002; Toccalino and others, 2010). The need to better understand these co-occurring compounds has increased, and an emerging area of science has begun to assess the potential effects of mixtures in the environment (Hertzberg and MacDonell, 2002; Agency for Toxic Substances and Disease Registry, 2004; U.S. Environmental Protection Agency, 2007). This study was designed to identify those unique mixtures of anthropogenic organic compounds (AOCs) that are most commonly detected in source water derived from rivers and groundwater.

Few studies have described the occurrence of AOCs in source water derived from rivers and groundwater. This study focuses on characterizing the occurrence of AOCs in source water derived from either rivers or groundwater. The occurrence of AOCs in rivers has been described, in part,

by Gilliom and others (1985), Gilliom and others (2006), Westrick (1990), and Kolpin and others (2002); some of these studies were synoptic, focused on ambient streams in different land-use settings, whereas other studies involved targeted sampling of rivers with a greater likelihood of detecting certain compounds. However, these studies did not focus on water specifically used for drinking water, and the sites sampled for these studies were not near CWS intakes. The occurrence of AOCs in groundwater has been documented, in part, by Westrick and others (1984), U.S. Environmental Protection Agency (2002), Gilliom and others (2006), and Zogorski and others (2006).

During 2002–12, the U.S. Geological Survey's (USGS's) National Water-Quality Assessment (NAWQA) Program completed studies at select CWSs across the United States (Delzer and Hamilton, 2007). The primary objective of these studies, termed Source Water-Quality Assessments (SWQAs), was to characterize the occurrence of a large number of predominantly unregulated AOCs in source water of CWSs. Kingsbury and others (2008) and Hopple and others (2009) summarized initial findings from this study for surface water and groundwater, respectively. This report summarizes source-water results for the entire 10-year study for which samples were collected during 2002–10.

The laboratory analytical methods used in this study attain relatively low minimum detection levels—commonly 100 to 1,000 times lower than State and Federal standards and guidelines for protecting water quality. Detections, therefore, do not necessarily indicate a concern to human health but instead may identify emerging water-quality issues and can be used to track changes in occurrence and concentrations through time. This study is intended to complement existing Federal, State, and local drinking-water monitoring programs, which focus primarily on post-treatment compliance monitoring of compounds regulated by EPA in finished drinking water to meet requirements of the SDWA. This study also provides information for many compounds not included in other source-water and finished-water monitoring programs such as the UCMR (U.S. Environmental Protection Agency, 2008a) and the U.S. Department of Agriculture's Pesticide Data Program (U.S. Department of Agriculture, 2008). In addition, this SWQA study contributes to specific science goals and priorities of the USGS, which, in part, include assessment of environmental risk to public health and the quality of water used for drinking water, as important aspects of accounting for the freshwater resources of the Nation (U.S. Geological Survey, 2007a).

The primary purpose of this report is to characterize the most commonly occurring AOCs in source water of CWSs that withdraw water solely from surface water (rivers) or groundwater (supply wells). Source-water samples were collected during 2002–10 from 20 river intakes and 448 supply wells. Rivers were sampled approximately 16 times over the course of a year and supply wells were sampled once. Samples from all sites were analyzed for 265 compounds that included disinfection by-products, fumigant-related compounds, fungicides,

gasoline hydrocarbons, herbicides, insecticides, manufacturing additives, organic synthesis compounds, pavement- and combustion-derived compounds, personal-care products, plant- or animal-derived biochemicals, refrigerants and propellants, and solvents. An additional 3 herbicides and 16 herbicide degradates (appendix 1) were analyzed in samples collected from sites in areas where these compounds likely have been used based on agricultural land use. This report describes (1) the sites sampled in a national context; (2) the occurrence of AOCs in surface-water and groundwater source water; and (3) a comparison of results between surface water and groundwater. Compound concentrations are evaluated in a human-health context, when possible, through comparison to EPA MCLs and USGS Health-Based Screening Levels (HBSLs). Specific ancillary factors determined to be associated with the occurrence and concentrations of compounds in source water and the most frequently co-occurring compounds are presented. Lastly, the occurrence of the additional herbicide degradates and their parent herbicides are presented.

## Study Design and Methods

The CWSs selected for monitoring met several criteria for surface-water and groundwater sites. Sites were located in NAWQA study areas where data from this study can be compared to other data collected during 1992 through 2012 from other sites within those study areas. The CWSs ideally were single-source systems (either groundwater or surface water) with little to no blending of water from multiple sources, and larger systems were preferred. The type of water treatment, previous monitoring results, including those for compliance monitoring, and the type of land use in the watershed or near the supply wells were not considered in the selection process.

### Selection of Surface-Water Sites

A total of 20 surface-water sites were selected for monitoring during 2002–10 (table 1; fig. 1). Sites were located on free-flowing reaches of rivers. Systems withdrawing from reservoirs with extensive residence times (on the order of days) were excluded to remain consistent with other river studies conducted by the NAWQA Program. However, in all cases, streamflow in the river could be affected by releases from upstream reservoirs. The mean distance between the CWS river intake and an upstream reservoir was about 40 kilometers (km), where the farthest reservoir was more than 130 km upstream from the intake.

The CWSs supplied by surface water (specifically, rivers) in this study represent a range in size of population served and are fairly well distributed across the United States. Nineteen of the 20 CWSs supplied by surface water are categorized as large or very large water systems (Carter and others, 2010), meaning that they provide water to more than 10,001 and 100,001 people, respectively (U.S. Environmental Protection

Agency, 2012b). One CWS was small, serving between 501 and 3,300 people.

### Selection of Groundwater Sites

A total of 448 CWS supply wells were sampled during 2002–10 as part of 30 independent groundwater studies (table 1; fig. 1). About 15 CWS wells were sampled for each groundwater study. The highest producing wells in each CWS typically were prioritized for sampling because these wells commonly have the largest contributing areas. Annual production data obtained from the CWSs were used to characterize withdrawals from the wells. In some cases, annual production data for individual wells were not available, so production volume for a well field or pumping center was used. Quartiles of production volumes were calculated among individual wells or pumping centers in a study, and 15 CWS wells were randomly selected from those in the top quartile. For CWSs where the top quartile did not contain enough wells or pumping centers for a random selection of 15 wells, a larger group of wells (for example, those in the upper two quartiles of production volume) was used for the random selection.

Selected wells were at least 1 km apart to minimize overlapping contributing areas. In general, wells sampled in this study are considered susceptible to anthropogenic contamination because of the relatively high pumping rates [generally greater than 32 liters per second (L/s)] and correspondingly large contributing areas. The results of this study are, therefore, not necessarily representative of wells with relatively low pumping rates (less than 32 L/s).

In certain aquifer systems, some of the highest-producing CWS wells were located near surface-water bodies, which could result in induced infiltration of surface water to the wells. The wells with this possible connection to rivers (groundwater under the influence of surface water) were avoided. Similarly, CWS wells in coastal or bay areas with induced infiltration from seawater, and wells used for injection and subsequent withdrawal of artificial recharge also were excluded because water samples from these types of wells do not typically represent recharge from the land surface.

### Compounds Monitored

Compounds monitored were selected on the basis of known or potential human-health concerns, analytical capabilities, and whether the compounds typically are not monitored in source water or finished water (appendix 1). Some compounds without known human-health concerns, such as caffeine, were included as potential indicators or surrogates for compounds not monitored. Most of the 265 compounds monitored at all sites are not regulated in drinking water and typically are not monitored by CWSs; however, 37 compounds are monitored and do have an established EPA MCL for drinking water. In addition, 29 compounds included on the CCL3 were monitored. Several inorganic compounds were

**Table 1.** Summary of locations and source of supply for source-water samples collected during 2002–10.[*n*, number of study locations; NAWQA, National Water-Quality Assessment]

State	Source Water-Quality Assessment study (NAWQA study unit identifier)	River or principal aquifer system sampled
Surface water ( <i>n</i> =20)		
Georgia	Apalachicola-Chattahoochee-Flint River Basins (ACFB)	Chattahoochee River
North Carolina	Albemarle-Pamlico Drainage Basins (ALBE)	Neuse River
Massachusetts	Connecticut, Housatonic, and Thames River Basins (CONN)	Running Gutter Creek
Pennsylvania	Delaware River Basin (DELR)	Schuylkill River
Iowa	Eastern Iowa Basins (EIWA)	Iowa River
Utah	Great Salt Lake Basins (GRSL)	Provo River
Ohio	Lake Erie-Lake Saint Clair Drainages (LERI)	Maumee River
New Jersey	Long Island-New Jersey Coastal Drainages (LINJ)	Raritan River
Alabama	Mobile River Basin (MOBL)	TallaPoosa River
Massachusetts	New England Coastal Basins (NECB)	Merrimack River
Nevada	Nevada Basin and Range (NVBR)	Truckee River
Arkansas	Ozark Plateaus (OZRK)	White River
Maryland	Potomac River Basin and Delmarva Peninsula (PODL)	Potomac River
California	Sacramento River Basin (SACR)	Sacramento River
South Carolina	Santee River Basin and Coastal Drainages (SANT)	Back River
Colorado	South Platte River Basin (SPLT)	Cache la Poudre River
Texas	Trinity River Basin (TRIN)	Elm Fork Trinity River
Minnesota	Upper Mississippi River Basin (UMIS)	Mississippi River
Indiana	White and Great and Little Miami River Basins (WHMI)	White River
Oregon	Willamette Basin (WILL)	Clackamas River
Groundwater ( <i>n</i> =30)		
Louisiana	Acadian-Pontchartrain Drainages (ACAD)	Coastal Lowlands aquifer system
Arizona	Central Arizona Basins (CAZB)	Basin and Range basin-fill aquifers
Washington	Central Columbia Plateau/Yakima River Basin (CCYK)	Columbia Plateau basin-fill and basaltic-rock aquifers
Connecticut	Connecticut, Housatonic, and Thames River Basins (CONN)	Glacial deposits aquifer system
Iowa	Eastern Iowa Basins (EIWA)	Cambrian-Ordovician aquifer system
Florida	Georgia-Florida Coastal Plain (GAFL)	Floridan aquifer system (semiconfined and unconfined unit)
Utah	Great Salt Lake Basins (GRSL)	Basin and Range basin-fill aquifers
Nebraska	High Plains Regional Groundwater Study (HPGW)	High Plains aquifer
New York	Long Island-New Jersey Coastal Drainages (LINJ)	Northern Atlantic Coastal Plain aquifer system
Illinois	Lower Illinois River Basin (LIRB)	Sand and gravel aquifers (glaciated regions)
Mississippi, Tennessee	Mississippi Embayment (MISE)	Mississippi embayment aquifer system

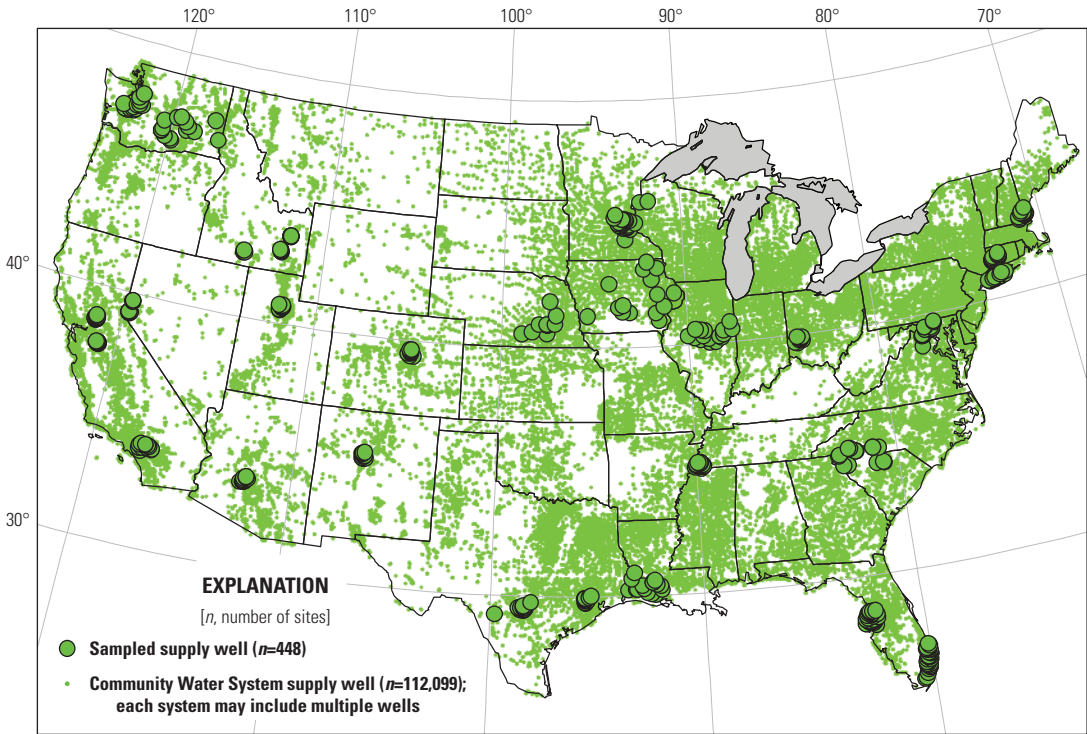
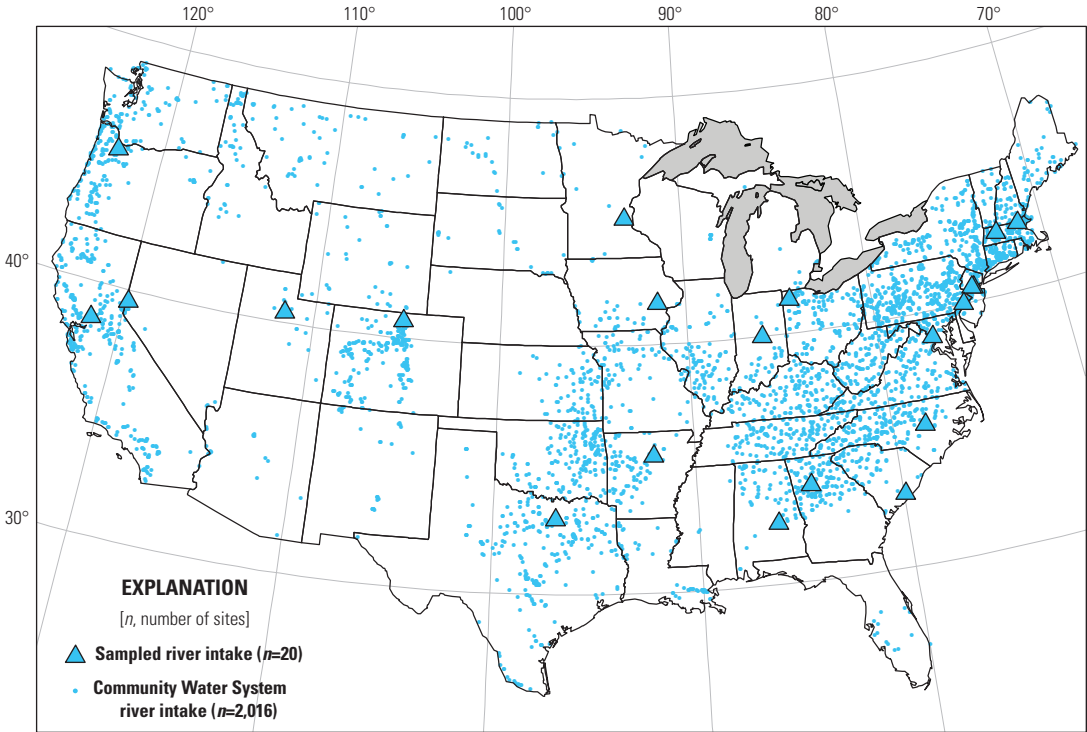
**Table 1.** Summary of locations and source of supply for source-water samples collected during 2002–10.—Continued[*n*, number of study locations; NAWQA, National Water-Quality Assessment]

State	Source Water-Quality Assessment study (NAWQA study unit identifier)	River or principal aquifer system sampled
Groundwater ( <i>n</i> =30)—Continued		
New Hampshire	New England Coastal Basins (NECB)	New England crystalline-rock aquifers
Nevada	Nevada Basin and Range (NVBR)	Basin and Range basin-fill aquifers
Maryland, Virginia	Potomac River Basin and Delmarva Peninsula (PODL)	Piedmont and Blue Ridge crystalline-rock aquifers
Washington	Puget Sound Basin (PUGT)	Puget Sound aquifer system
New Mexico	Rio Grande Valley (RIOG)	Rio Grande aquifer system
California	Sacramento River Basin (SACR)	Central Valley aquifer system
California	Santa Ana Basin (SANA)	California Coastal Basin aquifers
California	San Joaquin-Tulare Basins (SANJ)	Central Valley aquifer system
South Carolina	Santee River Basin and Coastal Drainages (SANT)	Piedmont and Blue Ridge crystalline-rock aquifers
Texas	South-Central Texas (SCTX)	Edwards-Trinity aquifer system
Florida	Southern Florida Drainages (SOFL)	Biscayne aquifer
Florida	Southern Florida Drainages (SOFL)	Surficial aquifer system
Colorado	South Platte River Basin (SPLT)	Denver Basin aquifer system
Texas	Trinity River Basin (TRIN)	Coastal Lowlands aquifer system
Minnesota, Wisconsin	Upper Mississippi River Basin (UMIS)	Cambrian-Ordovician aquifer system (Prairie du Chien Jordan aquifer)
Minnesota, Wisconsin	Upper Mississippi River Basin (UMIS)	Glacial deposits aquifer system
Idaho	Upper Snake River Basin (USNK)	Snake River Plain basaltic-rock aquifers
Idaho	Upper Snake River Basin (USNK)	Snake River Plain basin-fill aquifers
Ohio	White and Great and Little Miami River Basins (WHMI)	Glacial deposits aquifer system

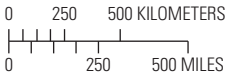
considered for monitoring but were not included because they typically are monitored by CWSs and, thus would not have provided new information. Additionally, only compounds that could be analyzed using USGS approved analytical methods (appendix 1) were considered for monitoring.

Of the 295 compounds initially monitored, 11 were removed because of observed systematic contamination, analytical variability, or because the compound was no longer analyzed by current (2014) USGS analytical methods. Nineteen herbicides and herbicide degradates were only sampled at select sites. The remaining 265 compounds monitored at all sites were grouped into 13 categories on the basis of their primary use or source. The number of compounds in each of the 13 categories (hereafter termed “use groups”) varies, ranging from 3 to 68 (table 2). About one-half of the compounds monitored are pesticides, which include herbicides and herbicide degradates, insecticides and insecticide degradates, and fungicides and fungicide degradates. About

90 volatile organic compounds (VOCs) were categorized in six use groups, including disinfection by-products; fumigant-related compounds; gasoline hydrocarbons, oxygenates, and oxygenate degradates; organic synthesis compounds; refrigerants and propellants; and solvents. Pesticides and VOCs have been monitored by the NAWQA Program since its inception (1991); however, most of the compounds in the remaining four use groups have not been monitored previously by the NAWQA Program (Gilliom and others, 2006; Zogorski and others, 2006). These use groups include personal-care and domestic-use products, such as triclosan (an anti-bacterial agent in many hand soaps), detergent metabolites, and fragrance compounds; manufacturing additives, such as plasticizers and fire retardants; pavement- and combustion-derived compounds, which are predominantly polynuclear aromatic hydrocarbons (PAHs); and plant- or animal-derived biochemicals, such as cholesterol.



Base modified from U.S. Geological Survey digital data, 1990, 1:2,000,000  
Albers Equal Area Conic projection  
Standard Parallels: 29°30'N and 45°30'N  
Central Meridian 96°00'W  
Horizontal coordinate information referenced to the  
North American Datum of 1983 (NAD 83)



**Figure 1.** General locations of sampled sites and all community water system sites derived from the Public-Supply Database. *A*, river intakes, and *B*, supply wells (data downloaded in 2010 from the U.S. Environmental Protection Agency's Safe Drinking Water Information System; Curtis V. Price, U.S. Geological Survey, written commun., 2012).

## 8 Anthropogenic Organic Compounds in Source Water of Select Community Water Systems in the United States, 2002–10

**Table 2.** Primary use groups for compounds analyzed in source water.

Primary use or source group	Description	Number of compounds in group for samples analyzed
Disinfection by-products	Trihalomethanes, (poly)haloacetic acids and other compounds that are produced from the transformation of organic compounds during the disinfection of water and wastewater through chlorination, ozonation, or other chemical methods.	4
Fumigant-related compounds	Chemicals that may be present in commercial fumigant products, which produce a gas, vapor, fumes, or smoke intended to destroy, repel, or control unwanted organisms such as insects, bacteria, or rodents. These include fumigant active ingredients, as well as their degradates and their manufacturing by-products.	9
Fungicides and fungicide degradates	Pesticides that are used to kill unwanted fungi.	9
Gasoline hydrocarbons, oxygenates, and oxygenate degradates	Gasoline hydrocarbons are straight, branched, and (or) cyclic organic compounds that are highly volatile, contain only carbon and hydrogen atoms, and are common ingredients in gasoline and other petroleum products. Among these compounds, BTEX (benzene, toluene, ethylbenzene, and xylene) compounds are among those present in the greatest proportions in gasoline. Oxygenates such as methyl <i>tert</i> -butyl ether (MTBE) are compounds that contain only carbon, hydrogen, and oxygen atoms and are commonly added to gasoline to improve the efficiency of combustion. Oxygenate degradates are formed during the production, storage, release, or use of gasoline oxygenates or following their release into the environment.	27
Herbicides and herbicide degradates	Pesticides designed to kill unwanted plants (herbicides) and compounds produced from the transformation of the parent herbicide following application (degradates).	68
Insecticides and insecticide degradates	Pesticides designed to kill unwanted insects (insecticides) and compounds produced from the transformation of the parent insecticide following application (degradates).	57
Manufacturing additives	Compounds used in commercial formulations of chemical products in order to improve the effectiveness of the product, including plasticizers (to increase the flexibility of plastics), fire retardants, corrosion inhibitors, and pesticide adjuvants.	6
Organic synthesis compounds	Chemicals that are used as precursors in the manufacture of other organic compounds. Chloroethylene (vinyl chloride), for example, is an organic synthesis compound used to produce polyvinyl chloride (PVC) plastics.	18
Pavement- and combustion-derived compounds	Organic substances, such as polynuclear aromatic hydrocarbons (PAHs), that are derived from either (1) the materials used to construct and seal parking lots and other paved surfaces, or (2) the combustion of other non-halogenated organic compounds, most commonly gasoline, oil, coal, and other fossil fuels.	5
Personal-care and domestic-use products	Compounds that are present in commercial products sold for personal or residential use, such as fragrances, pharmaceuticals, insect repellants, dyes, detergents, disinfectants, shampoos, and chemicals used in fire extinguishers.	22
Plant- or animal-derived biochemicals	Naturally occurring compounds that are produced by plants or animals, either through direct biosynthesis or through the metabolic alteration of compounds ingested or taken up from other sources. These compounds are predominantly unsaturated solid alcohols of the steroid group naturally occurring in fatty tissues of plants and animals and present in animal fecal material.	5
Refrigerants and propellants	Volatile compounds that are used for commercial or domestic refrigeration, as blowing agents in the manufacture of packaging and other highly porous materials, or for dispensing other substances from spray cans and other aerosol delivery devices.	3
Solvents	Compounds that are used to dissolve other substances. Two of the more common solvents are trichloroethene (TCE) and perchloroethene (PCE).	32
<b>Total number of compounds</b>		<b>265</b>

## Sample Collection and Protocols

Source water and quality-control samples were collected and processed following established USGS sampling protocols (U.S. Geological Survey, variously dated). Surface-water samples from rivers were collected monthly with additional samples collected during selected flow conditions when water quality could change quickly or when concentrations or the number of compounds expected to occur were maximized. These samples were collected from the river as close as practical to the drinking-water intake. Groundwater samples were collected once at the wellhead of the supply well before any treatment such as chlorination.

## Analytical Methods

Samples were analyzed using USGS approved analytical methods at the USGS National Water Quality Laboratory (NWQL) in Lakewood, Colorado, including gas chromatography/mass spectrometry (GC/MS) and high-performance liquid chromatography/mass spectrometry (HPLC/MS). Samples collected for VOC analyses were chilled upon collection. One VOC analytical method required additional preservation using 1:1 hydrochloric acid to achieve a pH of 2, whereas a second analytical method did not require the addition of hydrochloric acid. Samples for both VOC analytical methods were analyzed by purge and trap GC/MS (Connor and others, 1998; Rose and Sandstrom, 2003). Samples for analyses of pesticides and other semivolatile compounds were filtered in the field through a 0.7-micron baked glass-fiber filter and chilled. These samples were extracted at the NWQL on solid-phase extraction cartridges to concentrate the analytes from the filtered samples. The solid-phase extraction cartridges then were eluted with a solvent, and the extracts were analyzed by either GC/MS or HPLC/MS methods (Zaugg and others, 1995, 2002; Lindley and others, 1996; Furlong and others, 2001; Sandstrom and others, 2001; Madsen and others, 2003). At a subset of sites, an additional sample was collected for the analysis of 3 herbicides and 16 herbicide degradates. These samples were analyzed using HPLC/MS by the USGS Organic Geochemistry Research Group Laboratory, in Lawrence, Kansas (Lee and Strahan, 2003).

The analytical methods used at the NWQL and Organic Geochemistry Research Group Laboratory allow for the identification and quantification of compounds at low concentrations, in some cases as low as a few parts per trillion. Each analytical method has different ranges in sensitivity for its suite of analytes. Thus, the laboratory reporting levels (LRLs) for the compounds analyzed span four orders of magnitude, from 0.002 to 8.0 micrograms per liter ( $\mu\text{g/L}$ ) with a median of 0.04  $\mu\text{g/L}$ . Some reported concentrations are qualified as estimated (indicated with an “E”), which means the identification of the compound is reliable, but the concentration has greater uncertainty than unqualified concentrations reported for the same compound. These concentrations are estimated for one

of several reasons: (1) they are less than the lowest calibration standard; (2) the sample matrix interfered with measurement of the compound; (3) surrogates added to the sample indicated poor performance during the analysis; or (4) the compound consistently has poor recoveries, and therefore, concentrations are always reported as estimated.

The sensitivity of analytical methods can affect the calculated detection frequencies of the compounds monitored in this study. Compounds with low LRLs likely will be detected more commonly than those with high LRLs, given equal concentration distributions in the environment. To compare detection frequencies among compounds, a common assessment level of 0.05  $\mu\text{g/L}$  was applied to the concentration data to account for the different LRLs. The use of a common assessment level enables comparisons of the occurrence of multiple compounds by reducing potential bias resulting from certain compounds having greater analytical sensitivity than others. In this report, a common assessment level of 0.05  $\mu\text{g/L}$  was used. Seventy-five percent of all compounds analyzed have a LRL of 0.05  $\mu\text{g/L}$  or less. Analytical results for compounds detected in source water were evaluated both with and without an assessment level. In general, for comparisons of the occurrence between one compound and another compound, a common assessment level was used and any concentration less than or equal to 0.05  $\mu\text{g/L}$  was considered less than the LRL (that is, treated as a nondetected concentration). However, for comparisons of the occurrence of an individual compound between multiple locations, or for comparisons of the occurrence of one use group in source-water derived between surface water and groundwater, no assessment level was used, and all concentrations, including those qualified as estimated, were evaluated.

## Statistical Methods

The rank sum test, described by Helsel and Hirsch (2002), was used to compare surface water and groundwater concentrations. A threshold significance level ( $p$ -value) of 0.05 was used. A  $p$ -value less than 0.05 indicates that the test is significant. The  $p$ -value of 0.05 is a commonly used significance level (Sokal and Rohlf, 1995).

## Quality Assurance

Quality-assurance/quality-control samples collected for SWQA studies include equipment blanks, field blanks, source solution blanks, replicate samples, and finished-water matrix spikes. The various blank samples consisted of nitrogen-purged organic-free blank water. Equipment blanks typically are collected in a laboratory setting using the same sampling equipment used to collect environmental samples and typically are collected in a controlled environment before the environmental samples are collected. Equipment blanks are used to evaluate the cleanliness of sampling equipment before use. Field blanks are collected at or near sampling sites and are processed in the field in the same manner as

environmental samples. Field blanks are used to evaluate potential sample contamination from sampling equipment, cleaning procedures, the atmosphere, and shipment to the laboratory. Source solution blanks are used to determine the presence or absence of compounds in the water used to clean equipment and process equipment and field blanks. The various blank samples also provide information on contamination during shipment. Replicate samples measure the combined precision of sampling and laboratory analyses. The various blanks and replicates are summarized by Carter and others (2010). Matrix spike samples, which provide information about compound recoveries, were reported by Valder and others (2011).

Data from all source-water and quality-control samples collected by each SWQA were reviewed to evaluate potential bias (primarily systematic contamination) associated with sample collection, processing, transportation, and analysis. A review of all quality-control data as a whole along with the associated environmental data is important because the small number of samples collected in each study area generally is not adequate to characterize the full magnitude of potential bias. A larger dataset that covers the entire period of sample collection for SWQA studies provides greater insight to possible systematic errors that bias sample results (Carter and others, 2010).

Data for 11 AOCs were removed from this dataset because of systematic contamination, analytical variability, or because the compound was no longer analyzed. Phenol was detected frequently in field and laboratory blanks and at concentrations comparable to concentrations measured in environmental samples; thus, concentrations for phenol were removed from the dataset. Studies conducted by the NWQL (Mark Sandstrom, USGS National Water Quality Laboratory, oral commun., 2005) indicated that samples can be contaminated if *N,N*-diethyl-*meta*-toluamide (DEET) is used by sampling personnel. The frequent detection of DEET in field blanks caused uncertainty in the quality of DEET concentrations in environmental samples (Carter and others, 2010); thus, DEET was removed from the dataset. Three compounds—benzophenone, isophorone, and *para*-nonylphenol—were detected frequently in field blanks because of the presence of these compounds in the pH buffer (Trizma) obtained from the vendor. Because Trizma is only added to finished water samples containing free chlorine and not source-water samples, the quality of data for benzophenone, isophorone, and *para*-nonylphenol is not fully understood. Additionally, in the blank samples, concentrations were comparable to concentrations measured in environmental samples (Carter and others, 2010); thus, concentrations for benzophenone, isophorone, and *para*-nonylphenol were removed from the dataset. Laboratory analyses of bisphenol A and pentachlorophenol produced unreliable data starting in March 2005 (Dave Reppert, USGS National Water Quality Laboratory, written commun., 2010); thus, concentrations of bisphenol A and pentachlorophenol were removed from the dataset. Laboratory analysis of deethyldeisopropylatrazine, fonofos—oxygen analog, chlorothalonil, and 3-ketocarbocofuran

performed below the NWQL standards, and thus are no longer analyzed and were removed from the dataset.

For compounds detected in 50 percent or more of an individual SWQA's field blanks, all environmental and quality-control data for those compounds for that study area were removed from the dataset (Carter and others, 2010). After these concentrations were removed, compounds detected in 5 percent or more of all remaining field-blank samples were evaluated, and all detections of those compounds in environmental samples that were less than or equal to the highest blank concentration were censored by coding environmental concentrations with a "C<" and by changing the concentration value to the highest blank concentration. Compounds coded as "C<" were not included in any analyses herein. Data used in analyses are documented in Carter and others (2010).

## Human-Health Benchmarks Used for Screening-Level Assessments

Where a river (surface water) was the source of the drinking water, individual and annual mean concentrations of regulated compounds were compared to MCLs (U.S. Environmental Protection Agency, 2006a), and annual mean concentrations of unregulated compounds—those without EPA MCLs—were compared to HBSLs (Toccalino, 2007; Toccalino and others, 2008), when available. In this study, annual mean concentrations were calculated for each compound for each site. At most sites, samples were collected for about a 12-month period, but in some cases, the sampling period was somewhat longer or shorter than 12 months. Results for all samples for a particular site were used for calculating the annual mean concentration, and a value of one-quarter of the LRL was used when a compound was not detected. For plotting purposes, the median concentrations of the annual mean river concentrations for each site were used for comparison to human-health benchmarks.

Where a supply well (groundwater) was the source of the drinking water, individual concentrations of compounds were compared to MCLs and HBSLs, when available. Comparisons to human-health benchmarks were used in this report to identify concentrations of potential human-health concern and to provide an initial perspective on the potential importance of the AOCs detected.

Of the 265 compounds monitored in this study, 37 compounds have an established EPA MCL (U.S. Environmental Protection Agency, 2006a) and 123 compounds have an HBSL (Toccalino and others, 2008). Health-Based Screening Levels have not been developed for the remaining 105 unregulated compounds because of insufficient toxicity information. Therefore, the potential human-health significance of these 105 compounds cannot be evaluated at this time (Toccalino and others, 2006).

Maximum Contaminant Levels are legally enforceable EPA drinking-water standards that set the maximum permissible level of a compound in water that is delivered by public



water systems (U.S. Environmental Protection Agency, 2013a). Maximum Contaminant Levels are applicable only to finished-water samples in the regulatory framework; however, an assessment of source-water concentrations in relation to benchmarks provides an indication to water-resource managers and CWSs of potential concerns in the absence of factors such as water treatment and distribution. For rivers, the permissible level (MCL), depending on the compound, may be defined in terms of a single sample concentration or in terms of a time-weighted mean concentration (Toccalino, 2007).

Health-Based Screening Levels are benchmark concentrations of compounds in water that, if exceeded, may be of potential concern for human health. Health-Based Screening Levels are not regulatory standards, are not enforceable, and water systems are not required to monitor for any compounds for which HBSLs have been developed. Health-Based Screening Levels were developed collaboratively by the USGS, EPA, New Jersey Department of Environmental Protection, and Oregon Health and Science University (Toccalino and others, 2003). The HBSL values were developed using EPA Office of Water methodologies and EPA toxicity values, so they generally are comparable to EPA drinking-water guideline values such as Lifetime Health Advisory Levels and Risk Specific Level Concentrations (U.S. Environmental Protection Agency, 2012c). A  $10^{-6}$  to  $10^{-4}$  cancer risk level represents low and high HBSL values (Toccalino and others, 2008).

Concentrations of compounds in samples of source water were compared to human-health benchmarks as a screening-level assessment. This comparison identifies compounds with concentrations that approached or were greater than benchmarks to aid in assessing their potential relevance to human health. For these comparisons, benchmark quotient (BQ) values—the ratio of a concentration of a compound to its benchmark (MCL or HBSL)—were calculated. A BQ value greater than 1 represents a concentration greater than a benchmark. A BQ value greater than 0.1 can be used to identify compounds that may warrant additional monitoring (Toccalino and others, 2006). A threshold BQ of 0.1 (that is, one-tenth of the benchmark value) is consistent with various State and Federal practices (for example, U.S. Environmental Protection Agency, 1998). Monitoring for these compounds would enable analysis of trends in their occurrence and may provide an early indication if concentrations approach human-health benchmarks.

### Determination of Commonly Occurring Compounds

Although samples were analyzed for 265 compounds monitored at all sites, emphasis is placed on those found to commonly occur in source water. Commonly occurring compounds are defined herein as those that were detected in greater than or equal to 1 percent of samples using an assessment level of 0.05  $\mu\text{g/L}$  or when a compound was detected in greater than or equal to 10 percent of samples at no assessment level. By this definition, 71 compounds were identified

in surface water (table 3). Of these 71 compounds, 16 had the same detection frequency with and without the application of a common assessment level of 0.05  $\mu\text{g/L}$ , such as tri(2-butoxyethyl)phosphate (table 3; appendix 2). These 16 compounds have a median LRL that is greater than 0.05  $\mu\text{g/L}$ , and all detected concentrations were greater than that concentration. The 71 compounds represent 12 of the 13 use group categories (table 2); the refrigerants and propellants group was the only use group with no detections (appendix 2).

Twenty-eight commonly occurring compounds were identified in groundwater. Of these 28 compounds, 3 had the same detection frequency with and without the application of a common assessment level of 0.05  $\mu\text{g/L}$  (table 3; appendix 3) because the LRL for the 3 compounds is greater than 0.05  $\mu\text{g/L}$ . The 28 compounds represent seven use groups: disinfection by-products; gasoline hydrocarbons, oxygenates, and oxygenate degradates; herbicides and herbicide degradates; organic synthesis compounds; personal-care and domestic-use products; refrigerants and propellants; and solvents.

### Determination of Mixtures Used to Summarize Compound Co-Occurrence

A mixture occurrence analysis for the AOCs was done using methods used by Squillace and others (2002); J.C. Scott (U.S. Geological Survey, written commun., March 2011); DeSimone (2009); and Toccalino and others (2010). These methods define “unique mixtures” as specific combinations of two or more compounds in a given sample, regardless of the presence or absence of additional compounds in the same sample. By this definition, any environmental sample with hundreds of analyte concentrations could have thousands of unique combinations of mixtures present.

## Characterization of Community Water Systems and Sites Sampled for Anthropogenic Organic Compounds

Selected ancillary information was generated for CWSs throughout the conterminous United States and for the 20 river intakes and 448 CWS supply wells sampled by the USGS in this study to characterize sampled sites in a national context. An extract of the EPA Safe Drinking Water Information System (SDWIS) (U.S. Environmental Protection Agency, 2012b) was used to develop spatially derived and system-specific ancillary data. The SDWIS is a dataset that EPA aggregates from information submitted by the States. Before this study, the USGS, in cooperation with EPA, developed the Public Supply Database (PSDB) (U.S. Environmental Protection Agency, 2005; U.S. Environmental Protection Agency, 2012b; Curtis V. Price, U.S. Geological Survey, written commun., 2012), which integrates information available from active

**Table 3.** Summary of commonly occurring compounds in surface water ( $n=71$ ) and groundwater ( $n=28$ ).

[CASRN, Chemical Abstracts Service Registry Number; MCPA, (4-chloro-2-methylphenoxy)-acetic acid; %, percent; --, no information available; µg/L, micrograms per liter]

CASRN <sup>a</sup>	Compound name	Detection frequency criteria met to be considered a commonly occurring compound
		Surface water
95–63–6	1,2,4-Trimethylbenzene	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
106–46–7	1,4-Dichlorobenzene ( <i>p</i> -dichlorobenzene)	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
94–75–7	2,4-D	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
1928–38–7	2,4-D methyl ester	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
2163–68–0	2-Hydroxyatrazine	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
95–76–1	3,4-Dichloroaniline	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
360–68–9	3- <i>beta</i> -Coprostanol <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
136–85–6	5-Methyl-1 <i>H</i> -benzotriazole <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
34256–82–1	Acetochlor	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
67–64–1	Acetone (2-propanone) <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
21145–77–7	Acetyl hexamethyl tetrahydronaphthalene (AHTN)	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
15972–60–8	Alachlor	Detected in less than 1% of samples at an assessment level of 0.05 µg/L but detected in more than 10% of samples at no assessment level.
84–65–1	Anthraquinone	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
1912–24–9	Atrazine	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
17804–35–2	Benomyl	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
71–43–2	Benzene	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
83–46–5	<i>beta</i> -Sitosterol <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
19466–47–8	<i>beta</i> -Stigmastanol <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
75–27–4	Bromodichloromethane	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
75–25–2	Bromoform <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
58–08–2	Caffeine	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
76–22–2	Camphor	Detected in less than 1% of samples at an assessment level of 0.05 µg/L but detected in more than 10% of samples at no assessment level.
63–25–2	Carbaryl	Detected in less than 1% of samples at an assessment level of 0.05 µg/L but detected in more than 10% of samples at no assessment level.
90982–32–4	Chlorimuron-ethyl	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
108–90–7	Chlorobenzene	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
67–66–3	Chloroform	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
57–88–5	Cholesterol <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
156–59–2	<i>cis</i> -1,2-Dichloroethene	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
486–56–6	Cotinine	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
6190–65–4	Deethylatrazine	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
1007–28–9	Deisopropylatrazine	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
--	Desulfinylfipronil	Detected in less than 1% of samples at an assessment level of 0.05 µg/L but detected in more than 10% of samples at no assessment level.
333–41–5	Diazinon	Detected in less than 1% of samples at an assessment level of 0.05 µg/L but detected in more than 10% of samples at no assessment level.
124–48–1	Dibromochloromethane <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
1918–00–9	Dicamba	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.
330–54–1	Diuron	Detected in 1% or more of samples at an assessment level of 0.05 µg/L.

**Table 3.** Summary of commonly occurring compounds in surface water ( $n=71$ ) and groundwater ( $n=28$ ).—Continued[CASRN, Chemical Abstracts Service Registry Number; MCPA, (4-Chloro-2-methylphenoxy)-acetic acid; %, percent; --, no information available;  $\mu\text{g/L}$ , micrograms per liter]

CASRN <sup>a</sup>	Compound name	Detection frequency criteria met to be considered a commonly occurring compound
		Surface water—Continued
100-41-4	Ethylbenzene	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
120068-37-3	Fipronil	Detected in less than 1% of samples at an assessment level of 0.05 $\mu\text{g/L}$ but detected in more than 10% of samples at no assessment level.
120067-83-6	Fipronil sulfide	Detected in less than 1% of samples at an assessment level of 0.05 $\mu\text{g/L}$ but detected in more than 10% of samples at no assessment level.
206-44-0	Fluoranthene	Detected in less than 1% of samples at an assessment level of 0.05 $\mu\text{g/L}$ but detected in more than 10% of samples at no assessment level.
1222-05-5	Hexahydrohexamethyl-cyclopentabenzopyran (HHCB)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
51235-04-2	Hexazinone	Detected in less than 1% of samples at an assessment level of 0.05 $\mu\text{g/L}$ but detected in more than 10% of samples at no assessment level.
81335-77-5	Imazethapyr	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
<i>m</i> : 108-38-3; <i>p</i> : 106-42-3	<i>m</i> - & <i>p</i> -Xylene	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
94-74-6	MCPA	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
1634-04-4	Methyl <i>tert</i> -butyl ether (MTBE)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-09-2	Methylene chloride	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
51218-45-2	Metolachlor	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
74223-64-6	Metsulfuron methyl <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
91-20-3	Naphthalene <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
26027-38-2	Nonylphenol, diethoxy- (total) <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
2315-61-9/ 51437-90-2	Octylphenol, diethoxy- (OPEO2)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
2315-67-5/ 51437-89-9	Octylphenol, monoethoxy- (OPEO1) <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
95-47-6	<i>o</i> -Xylene	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
106-44-5	<i>p</i> -Cresol	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
127-18-4	Perchloroethene (PCE; tetrachloroethene)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
1610-18-0	Prometon	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
709-98-8	Propanil	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
122-34-9	Simazine	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
5915-41-3	Terbutylazine	Detected in less than 1% of samples at an assessment level of 0.05 $\mu\text{g/L}$ but detected in more than 10% of samples at no assessment level.
994-05-8	<i>tert</i> -Amyl methyl ether (TAME)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-65-0	<i>tert</i> -Butyl alcohol <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
109-99-9	Tetrahydrofuran (1,4-epoxybutane) <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
108-88-3	Toluene	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
78-51-3	Tri(2-butoxyethyl)phosphate <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
115-96-8	Tri(2-chloroethyl)phosphate <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
79-01-6	Trichloroethene (TCE)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
55335-06-3	Triclopyr	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
3380-34-5	Triclosan	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .

**Table 3.** Summary of commonly occurring compounds in surface water ( $n=71$ ) and groundwater ( $n=28$ ).—Continued[CASRN, Chemical Abstracts Service Registry Number; MCPA, (4-Chloro-2-methylphenoxy)-acetic acid; %, percent; --, no information available;  $\mu\text{g/L}$ , micrograms per liter]

CASRN <sup>a</sup>	Compound name	Detection frequency criteria met to be considered a commonly occurring compound
		Surface water—Continued
77-93-0	Triethyl citrate	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
13674-87-8	Tris(dichlorisopropyl) phosphate	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
Groundwater		
71-55-6	1,1,1-Trichloroethane	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
76-13-1	1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-34-3	1,1-Dichloroethane	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-35-4	1,1-Dichloroethene	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
107-06-2	1,2-Dichloroethane (ethylene dichloride) <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
2163-68-0	2-Hydroxyatrazine	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
140-66-9	4- <i>tert</i> -Octylphenol	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
1912-24-9	Atrazine	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
25057-89-0	Bentazon	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-27-4	Bromodichloromethane	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-25-2	Bromoform	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-15-0	Carbon disulfide <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
56-23-5	Carbon tetrachloride	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
67-66-3	Chloroform	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
156-59-2	<i>cis</i> -1,2-Dichloroethene	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
6190-65-4	Deethylatrazine	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
124-48-1	Dibromochloromethane	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-71-8	Dichlorodifluoromethane (CFC-12)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
330-54-1	Diuron	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
51235-04-2	Hexazinone	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
1634-04-4	Methyl <i>tert</i> -butyl ether (MTBE)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
127-18-4	Perchloroethene (PCE; tetrachloroethene)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
1610-18-0	Prometon	Detected in less than 1% of samples at an assessment level of 0.05 $\mu\text{g/L}$ but detected in more than 10% of samples at no assessment level.
122-34-9	Simazine	Detected in less than 1% of samples at an assessment level of 0.05 $\mu\text{g/L}$ but detected in more than 10% of samples at no assessment level.
34014-18-1	Tebuthiuron	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
79-01-6	Trichloroethene (TCE)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-69-4	Trichlorofluoromethane (CFC-11)	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .
75-01-4	Vinyl chloride <sup>b</sup>	Detected in 1% or more of samples at an assessment level of 0.05 $\mu\text{g/L}$ .

<sup>a</sup>This report contains Chemical Abstracts Service Registry Numbers (CASRN)<sup>®</sup>, which is a Registered Trademark of the American Chemical Society. The CASRN online database provides the latest registry number information: <http://www.cas.org/>. Chemical Abstracts Service recommends the verification of the CASRNs through CAS Client Services<sup>SM</sup>.

<sup>b</sup>Compounds have the same detection frequency with and without an assessment level of 0.05  $\mu\text{g/L}$ .

systems and facilities in SDWIS with matched data stored in the USGS National Water Information System (NWIS). The PSDB includes a large list of 11,400 surface-water intakes and 144,232 supply wells. Many of these records represent SDWIS sites that are now inactive or destroyed, or represent other types of facilities such as conveyances (deliveries between water systems).

Surface-water intake locations were supplied to EPA to develop watershed polygons. These watershed polygons were, in turn, provided to USGS for verification. A detailed check of these watersheds yielded a set of 4,831 unique intake watersheds determined to have accurate delineations (Michael E. Wieczorek, U.S. Geological Survey, written commun., 2012). Of these unique intake watersheds, 2,016 were determined to represent intake locations on rivers, based on the facility name and whether the intake was included in the National Inventory of Dams to exclude lakes and reservoirs (Alexander and others, 1999). Of the 144,232 supply wells, a total of 112,099 wells were determined to be active CWS wells with valid latitude-longitude locations. These wells were buffered with a 500-meter (m) radius to create circular groundwater contributing area polygons surrounding each well. These 2,016 watersheds and 112,099 contributing areas are considered to represent the national population of river and supply well sites, respectively, supplying CWSs. Ancillary variables were characterized within their boundaries using the NAWQA Area-Characterization Toolbox (Price and others, 2010). Ancillary variables include population served, basin size, land use, population density, and recharge (table 4).

Overall, the source waters sampled as part of this study represent about 1 percent of all CWS river intakes and 0.4 percent of all CWS supply wells in the conterminous United States (fig. 1). Although comparatively few sites were sampled relative to the national population of sites, comparison of ancillary variables for sampled sites generally covered the range of the total distribution of the national population with the exception of population served and watershed size for river intakes.

The national distribution of population served for CWSs associated with the 2,016 river intakes as well as the population served for CWSs supplied by the 20 sampled intakes is shown on figure 2. Fifty percent of all systems serve a population greater than 5,900 persons. When comparing this to 20 sampled river intakes, 19 CWSs served more than 12,000 persons. This is a reflection of the study design, which specifically targeted larger CWSs for sampling. Similarly, comparing watershed size of sampled sites to the national distribution reveals that rivers with some of the largest watersheds were sampled (fig. 3A). This may be an artifact of targeting large CWSs serving populations near large rivers, which have large watersheds. The median watershed size of all 2,016 river intakes was 330.1 square kilometers (km<sup>2</sup>). Nineteen of the 20 sampled river intakes

had a watershed size greater than 1,000 km<sup>2</sup>; one river intake had a watershed size less than 10 km<sup>2</sup> (fig. 3A).

The surface-water and groundwater sites were characterized by the dominant type of land use within each watershed for river intakes and for contributing areas around each supply well (table 5). To put results from this study into context with the national distribution of river intakes and supply wells used by CWS, all of the sites were grouped into a national population of land-use quartiles. Three of the land-use categories within each of the 20 watersheds were compared to the total distribution of the national population. Urban, agricultural, and undeveloped land use within the 20 watersheds generally covered the range of the total distribution of the national population (fig. 3B, C, and D, respectively). Similarly, population density and recharge for the 20 watersheds reasonably cover the range of the national distribution (fig. 3E and F, respectively).

Comparison of ancillary variables for the contributing areas around the 448 supply wells, including population served, population density, urban and agricultural land use, and recharge, fully covered the range of the total distribution of the national population of 112,099 supply wells (figs. 4 and 5). The covered range of ancillary variables in these contributing areas may be more evenly distributed across the national distribution, in part, because of the larger number of wells sampled in comparison to the number of river intakes sampled.

Although this study was not designed as a comprehensive national-scale assessment of water supplying CWSs, the sites selected are considered to be representative of most systems in the Nation, with the exception of rivers supplying CWSs that serve small populations (less than 10,000) and that have a small watershed size (less than 1,000 km<sup>2</sup>). Overall, ancillary variables for watersheds of river intakes and for contributing areas of supply wells covered the range of the total distribution of the national population favorably. Although the number of river intakes and supply wells sampled is much smaller than the national dataset, observed patterns in water quality related to ancillary variables may still allow inferences to nonsampled river intakes and wells with similar ancillary conditions. Observed patterns in water quality related to ancillary factors may be used to estimate the number of nonsampled river intakes and supply wells with similar characteristics. For example, quartiles from the national population of ancillary data can be determined and sampled sites can be evaluated within each of the quartiles. Because the sampled sites are considered to represent the national population, water-quality determinations within each quartile may be used to infer the total number of nonsampled CWS sites within each quartile that may have similar ancillary conditions.

**Table 4.** Summary of ancillary variables characterized in each of 2,016 watersheds for river intakes and 112,099 contributing areas for supply wells used in relational analysis.

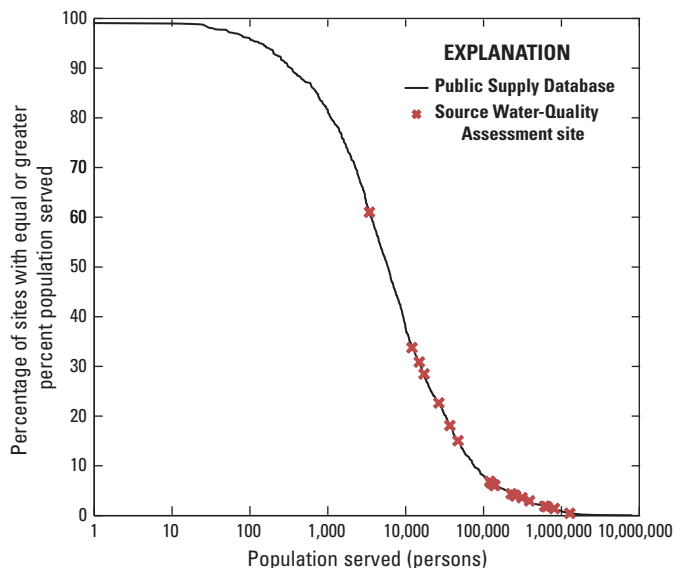
[EPA, U.S. Environmental Protection Agency; SDWIS, Safe Drinking Water Information System; km<sup>2</sup>, square kilometers; N/A, not applicable; NHDPPlus, National Hydrography Dataset (U.S. Environmental Protection Agency and U.S. Geological Survey, 2010); USGS, U.S. Geological Survey; mm/yr, millimeter per year]

Variable	Description	Units	Domain	Source resolution	Source
Population served	Population served (as reported in EPA SDWIS database)	Persons	Integer (null if not available)	N/A; (non-spatial data, reported by water system in SDWIS)	U.S. Environmental Protection Agency, 2012b; supplemented by data from Public Supply Database, Curtis V. Price, USGS (written commun., 2012).
Basin size <sup>a</sup>	Area calculated from drainage basin polygons	km <sup>2</sup>	Area values	N/A	Drainage basin polygons developed using NHDPPlus by Michael E. Wieczorek, USGS (written commun., 2012).
Classified land use	Land use re-classified from percentage land-use values.	N/A	Urban, mixed urban, agricultural, mixed agricultural, undeveloped, mixed	30-meter grid cells	Tabulated land-use percentages (see table 5).
Urban land	Urban (classes 21–24) <sup>b</sup>	Percent	0–100	30-meter grid cells	Homer and others, 2007.
Agricultural land	Agricultural (classes 81 and 82) <sup>c</sup>	Percent	0–100	30-meter grid cells	Homer and others, 2007.
Undeveloped land	All other land cover classes	Percent	0–100	30-meter grid cells	Homer and others, 2007.
Population density	Block group population density	Persons per km <sup>2</sup>	Continuous	100-meter grid	Radeloff and others, 2005 (based on Bureau of the Census, 2001).
Recharge	Estimated mean annual recharge	mm/yr	Continuous	1-kilometer grid cell	Wolock, 2003.

<sup>a</sup>Characterized only for river intakes.

<sup>b</sup>Class 21 = developed, open space; class 22 = developed, low intensity; class 23 = developed, medium intensity; class 24 = developed, high intensity.

<sup>c</sup>Class 81 = pasture/hay; class 82 = cultivated crops.



**Figure 2.** Distribution of population served for community water systems supplied by 2,016 river intakes in the conterminous United States compared to sampled river intakes.

## Occurrence of Anthropogenic Organic Compounds in Source Waters

Surface-water and groundwater samples collected at all river intakes and supply wells, respectively, were analyzed for 265 AOCs; however, emphasis is placed on those detected commonly in source water. An additional 3 herbicides and 16 herbicide degradates were studied at a subset of sites where these compounds likely have been used. Because the additional compounds were not monitored at all of the sites, they are described separately from the most commonly occurring compounds that were monitored at all sites. Between the years of 2002 through 2010, 16 surface-water samples at river intakes were collected over the course of a year and groundwater samples were collected once from each supply well during 2002–09. A total of 313 samples were collected from 20 river intakes and 448 groundwater samples were collected for 30 individual SWQA studies around the country.

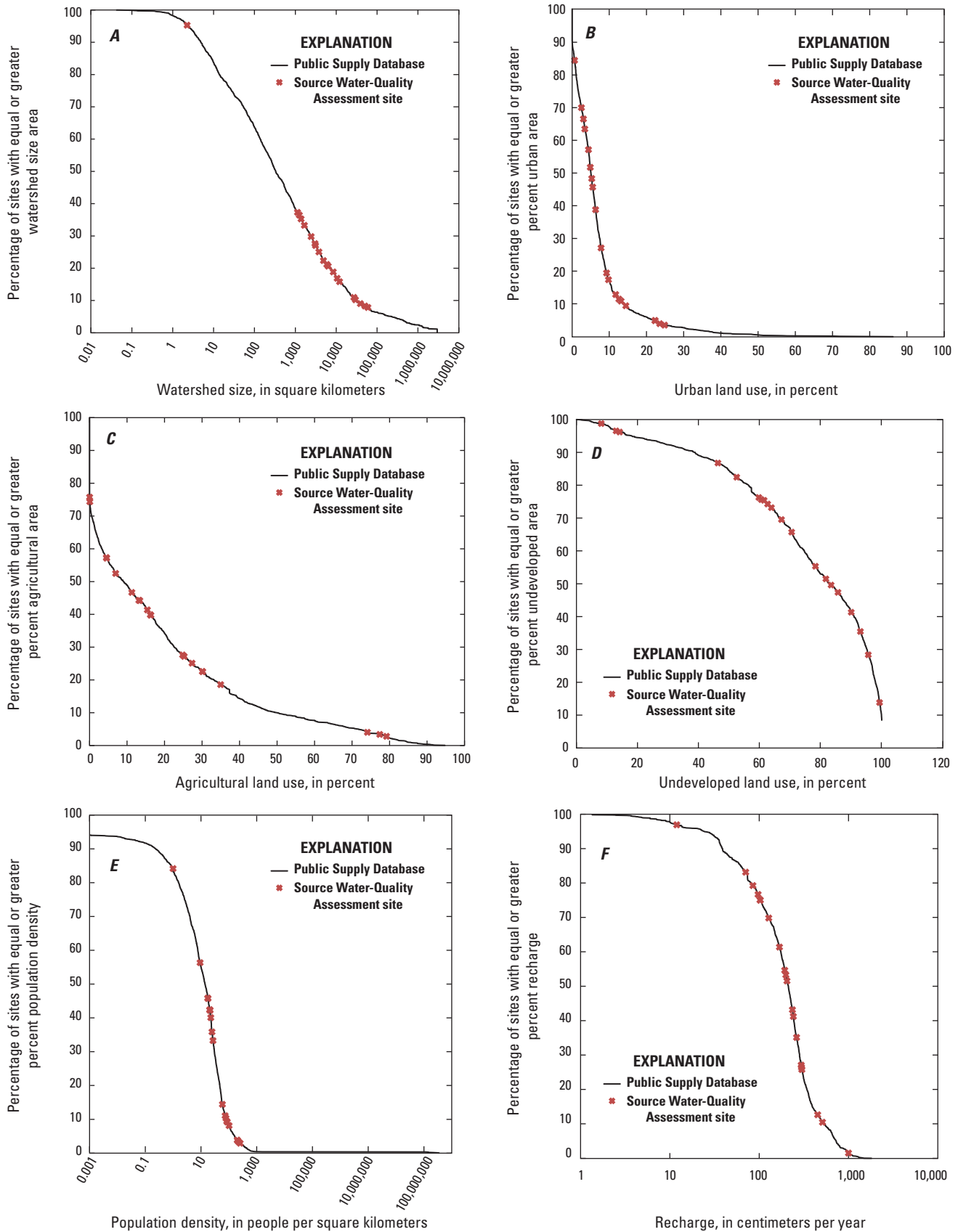
Compound occurrence is summarized in four sections: (1) occurrence in surface water; (2) occurrence in groundwater; (3) comparison of occurrence between surface-water and groundwater; and (4) additional herbicides and herbicide degradates. In general, the characterization of occurrence focuses on the most frequently occurring compounds (table 3) with and without an assessment level, comparison of concentrations to human-health benchmarks, factors that may affect occurrence, and unique mixtures that frequently co-occur in samples.

Compound occurrence was determined with and without an assessment level. An assessment level of 0.05  $\mu\text{g/L}$  was used herein to compare detection frequencies for individual compounds with different LRLs. Detection frequency depends on the LRL for each compound monitored. Thus, different detection frequencies for compounds with different LRLs may not represent true differences in water quality, but rather may only reflect differences in analytical sensitivity among the different compounds. Therefore, one approach to characterizing compound occurrence was the use of a common assessment level. Conversely, using no assessment level emphasizes the significance of low-level concentrations at which many of these compounds were detected. Detections of AOCs do not necessarily indicate a concern to human health but rather help to identify emerging issues and are useful to track changes in occurrence and concentrations through time. The frequency of detection for all 265 AOCs and the additional 19 herbicides and herbicide degradates for surface water and groundwater are summarized in appendixes 2 and 3, respectively, and the concentration data for the detected compounds are shown in appendixes 4 and 5, respectively.

Comparing source-water concentrations to human-health benchmarks helps to provide (1) some context for the results relative to human health and (2) some insight into which compounds merit additional study or monitoring. Although MCLs and HBSLs are not directly applicable to source-water samples, comparing concentrations of compounds in source water to human-health benchmarks is important because many of the compounds monitored may not be removed by water treatment processes unless specifically designed for their removal. In samples collected from rivers, both the individual concentrations and the annual mean concentrations for all compounds with a human-health benchmark were evaluated.

Occurrence information was further evaluated with respect to various ancillary factors, which may provide an improved understanding of compound occurrence. Ancillary factors included, in part, land use, population density, and population served. When applicable, additional ancillary factors specific to rivers and supply wells also were used in interpreting the occurrence of compounds found in samples.

A total of 313 and 448 rivers and groundwater samples, respectively, were included in the mixture analyses. Mixtures were examined in three categories: (1) an overall assessment of mixtures present in samples (that is, the number of compounds present in samples), (2) unique mixtures of specific compounds with an assessment level applied to the concentrations, and (3) unique mixtures of specific compounds without an assessment level. Because of the enormous (several million) number of combinations of unique mixtures of compounds in any given sample using no assessment level, only the 10 most frequently occurring mixture combinations are presented in this report.



**Figure 3.** Distribution of 2,016 river intakes compared to sampled river intakes. *A*, watershed size; *B*, urban land use within watershed; *C*, agricultural land use within watershed; *D*, undeveloped land use within watershed; *E*, population density within watershed; and *F*, recharge within watershed (modified from Wolock, 2003).



**Table 5.** Land-use classification (modified from Gilliom and others, 2006).

[>, greater than; ≤, less than or equal to; <, less than]

Land-use classification	Watershed land-use criteria
Agricultural (ag)	> 50 percent “ag” and ≤ 5 percent “ur”
Urban (ur)	> 25 percent “ur” and ≤ 25 percent “ag”
Undeveloped (un)	< 5 percent “ur” and ≤ 25 percent “ag”
Mixed	All other combinations of “ur”, “ag”, and “un”
Ur mixed	“Mixed” (as above) and percent “ur” > 20
Ag mixed	“Mixed” (as above) and percent “ag” > 50 and percent “ur” < 10

### Commonly Occurring Anthropogenic Organic Compounds in Surface Water

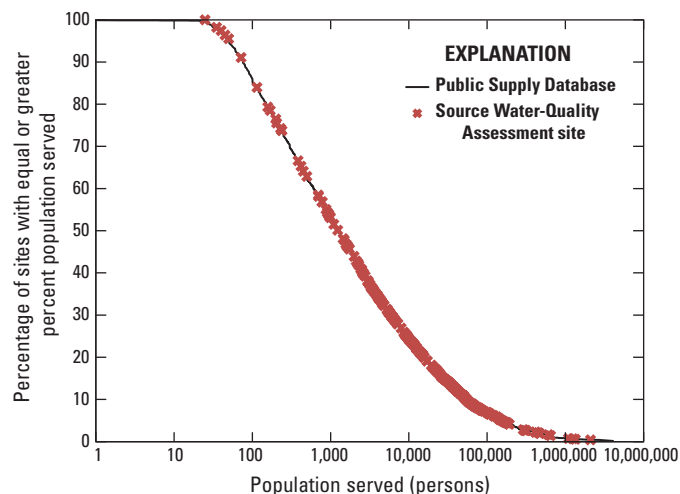
Ninety-eight (about 37 percent) of the 265 AOCs monitored at all sites were detected in one or more surface-water samples, and 167 AOCs (about 63 percent) were never detected using an assessment level of 0.05 µg/L (appendix 2). An assessment level (0.05 µg/L used herein) is necessary to compare detection frequencies of one compound to another because of the differing LRLs among compounds and through time. Commonly occurring compounds are defined as those that were detected in greater than or equal to 1 percent of samples using an assessment level of 0.05 µg/L or those compounds detected in greater than or equal to 10 percent of samples without an assessment level. This section focuses on compound occurrence in surface water. Concentrations are evaluated in more detail in the “Comparison of Surface-Water and Groundwater Occurrence” section.

Seventy-one compounds were found to commonly occur, as defined previously, in surface-water samples (fig. 6). Using the assessment level, 15 compounds were detected in more than 10 percent of samples. Of these 15 compounds, six were detected in 20 percent or more of samples: hexahydrohexamethylcyclopentabenzopyran (HHCB) (29.5 percent), chloroform (27.3 percent), atrazine (27.3 percent), tri(2-butoxyethyl) phosphate (23.8 percent), methyl *tert*-butyl ether (MTBE) (20.9 percent), and 2,4-D (20.4 percent). The most commonly occurring compound, HHCB, is commonly used in detergents and other personal-care products and has been found in both influent and effluent of wastewater-treatment plants in the United States and Europe (Bester, 2004; Phillips and others, 2005). Hexahydrohexamethylcyclopentabenzopyran is a synthetic musk fragrance used in items such as decorative cosmetics, shampoos, toilet soaps, household cleaners, and detergents (Api and Ford, 1999). Three of the most commonly occurring compounds—HHCB, chloroform, and

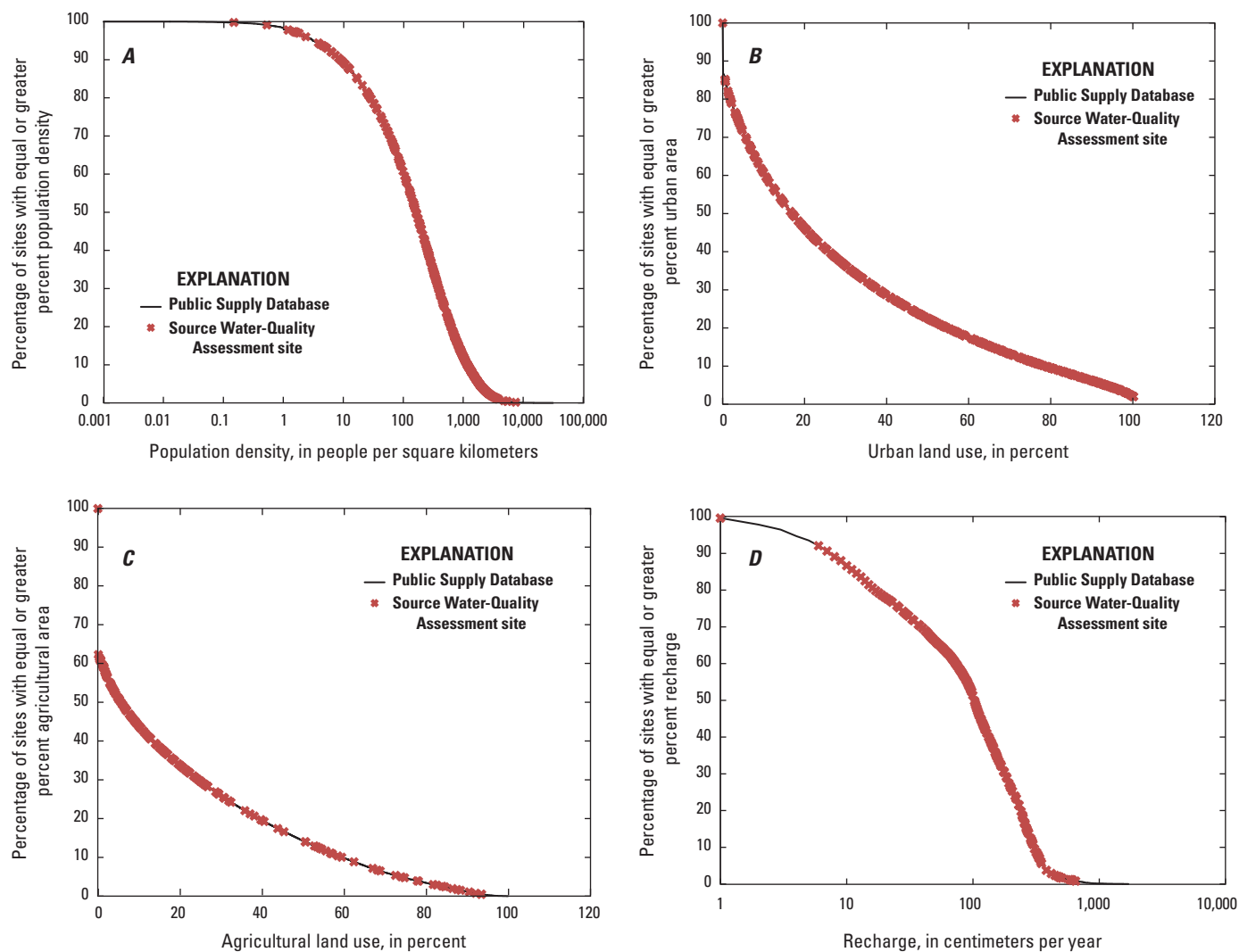
tri(2-butoxyethyl)phosphate—have been linked to influent and effluent of municipal and industrial wastewater discharge (Bester, 2004; Phillips and others, 2005; Ivahnenko and Barbash, 2004; Kolpin and others, 2002; Kingsbury and others, 2008). This highlights the importance of understanding discharges from wastewater-treatment plants and septic systems to surface waters used as a source of supply for CWSs. Atrazine, MTBE, and 2,4-D have each been linked to overland runoff and releases from leaking underground storage tanks (Gilliom and others, 2006; Zogorski and others, 2006; Rowe and others, 2007).

A wide variety of compounds were detected in surface-water samples. Compounds from 12 of the 13 use groups were found to commonly occur indicating that a wide variety of sources and pathways exist for these compounds to reach the rivers sampled. No compounds in the refrigerants and propellants group were detected in any surface-water samples. Compounds in the herbicides and herbicide degradates group were among the most commonly detected compounds followed by the gasoline hydrocarbons, oxygenates, and oxygenate degradates group and the personal-care and domestic-use products group (fig. 6).

Of the 71 commonly occurring compounds in surface-water samples, 22 compounds were herbicides and herbicide degradates. Their frequent detection is due to their widespread use compared to other compounds and may be an artifact of the larger number of herbicides analyzed in samples in comparison to other compounds. Previous studies indicate that herbicide degradates typically occur with their parent compounds at concentrations similar to or greater than concentrations of their parent compounds (Thurman and others, 1992; Kalkhoff and others, 1998; Gilliom and others, 2006). For many degradates, little is known about their occurrence or their effects on human health. With a few exceptions for herbicides and



**Figure 4.** Distribution of population served for community water systems supplied by 112,099 supply wells in the conterminous United States compared to sampled supply wells.



**Figure 5.** Distribution of 112,099 supply wells compared to sampled supply wells. *A*, population density within contributing area; *B*, urban land use within contributing area; *C*, agricultural land use within contributing area; and *D*, recharge within contributing area (modified from Wolock, 2003).

degradates with known common modes of action, drinking-water standards or human-health benchmarks are not available for most herbicide degradates. Several herbicide degradates, principally those of atrazine and 3,4-dichloroaniline (a degradate of diuron), were detected. Atrazine was the most frequently detected herbicide, detected in 27.3 percent of the samples at an assessment level of 0.05  $\mu\text{g/L}$ . Atrazine was detected in 69.7 percent of samples without an assessment level with concentrations ranging from 0.002 to 20.1  $\mu\text{g/L}$  and a median concentration of 0.03  $\mu\text{g/L}$ .

Ten gasoline hydrocarbons, oxygenates, and oxygenate degradates commonly occurred in surface-water samples. These compounds may be contributed to surface water from groundwater discharge, runoff from roads and parking lots, and watercraft that are used on these rivers or upstream reservoirs (Zogorski and others, 2006). Using an assessment level, MTBE was the most frequently detected compound in this use group (20.9 percent). Methyl *tert*-butyl ether is a

gasoline oxygenate first introduced in 1979 to replace lead as an octane enhancer (U.S. Environmental Protection Agency, 2013b). Methyl *tert*-butyl ether has been detected in drinking-water supplies throughout the country in previously published studies (Zogorski and others, 2006; Carter and others, 2006; U.S. Environmental Protection Agency, 2008b). Methyl *tert*-butyl ether was detected in 24.3 percent of samples without an assessment level with concentrations ranging from 0.03 to 3.4  $\mu\text{g/L}$  and a median concentration of 0.12  $\mu\text{g/L}$ . The maximum concentration was detected in only one sample at one site. The second highest concentration detected was 0.7  $\mu\text{g/L}$  at the same site.

Ten personal-care and domestic-use products commonly occurred. Hexahydrohexamethylcyclopentabenzopyran was the most frequently detected personal-care and domestic-use product (29.5 percent) using an assessment level, followed by caffeine (12.4 percent); nonylphenol, diethoxy- (total) (10.4 percent); and acetyl hexamethyl tetrahydronaphthalene

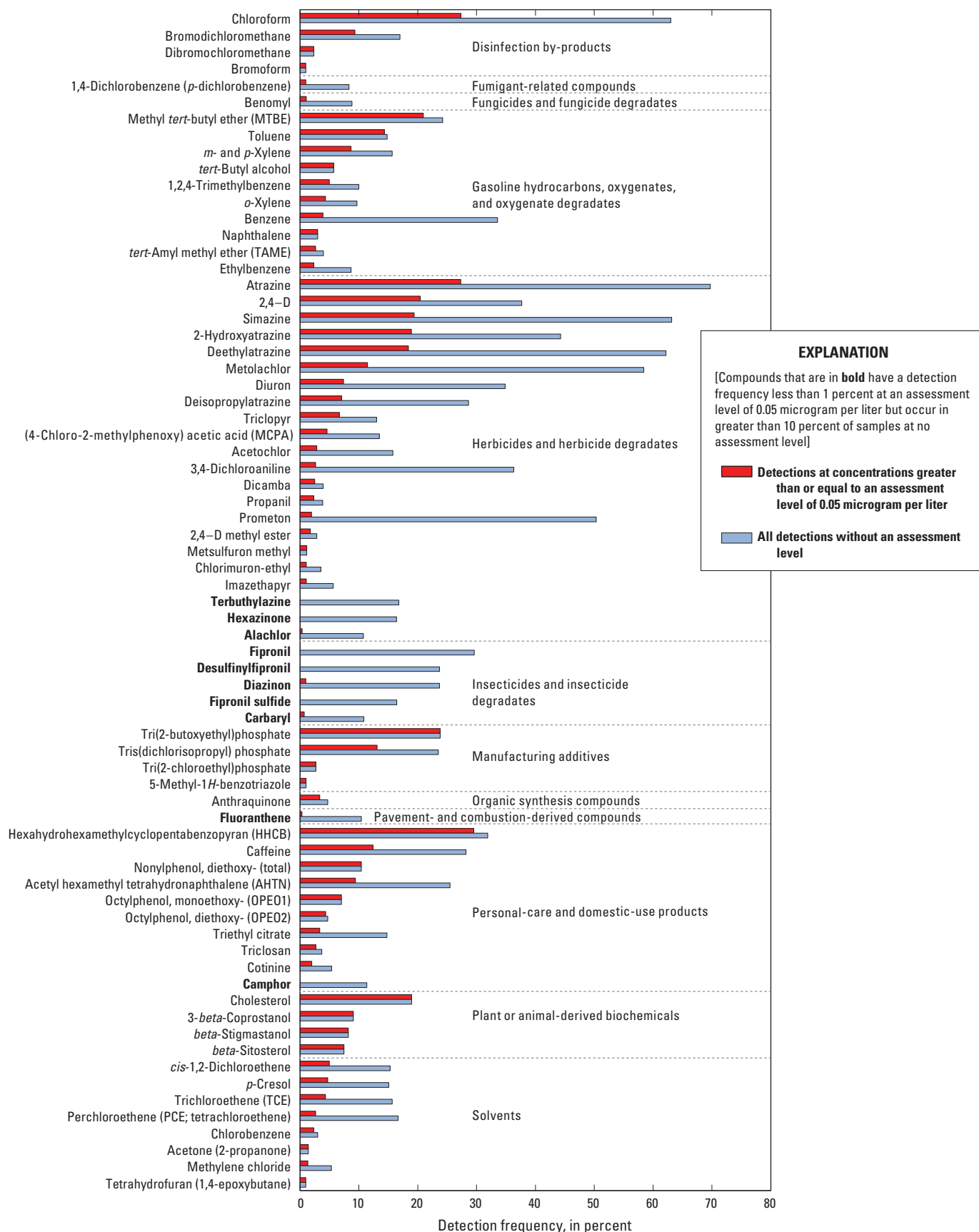


Figure 6. Commonly occurring compounds in source water derived from surface water.

(AHTN) (9.4 percent). Hexahydrohexamethylcyclopentabenzopyran was detected in 31.9 percent of samples without an assessment level with concentrations ranging from 0.05 to 0.26  $\mu\text{g/L}$  and a median concentration of 0.08  $\mu\text{g/L}$ . Caffeine was detected in 28.2 percent of samples without an assessment level with concentrations ranging from 0.01 to 0.28  $\mu\text{g/L}$  and a median concentration of 0.05  $\mu\text{g/L}$ . Nonylphenol, diethoxy-(total) was detected in 10.4 percent of samples without an assessment level with concentrations ranging from 0.47 to 6.6  $\mu\text{g/L}$  and a median concentration of 1.7  $\mu\text{g/L}$ . Acetyl hexamethyl tetrahydronaphthalene was detected in 25.5 percent of samples without an assessment level with concentrations ranging from 0.005 to 0.15  $\mu\text{g/L}$  and a median concentration of 0.04  $\mu\text{g/L}$ . Previously published studies have indicated that personal-care products may be introduced to rivers from treated wastewater discharge (Kingsbury and others, 2008).

Four of the 71 commonly occurring compounds were on the CCL3 (U.S. Environmental Protection Agency, 2012a): acetochlor, diuron, MTBE (described previously), and metolachlor. Acetochlor was detected in 15.8 percent of samples without an assessment level with concentrations ranging from 0.003 to 4.32  $\mu\text{g/L}$  and a median concentration of 0.012  $\mu\text{g/L}$ . Diuron was detected in 34.9 percent of samples without an assessment level with concentrations ranging from 0.002 to 0.47  $\mu\text{g/L}$  and a median concentration of 0.024  $\mu\text{g/L}$ . Metolachlor was detected in 58.4 percent of samples without an assessment level with concentrations ranging from 0.002 to 2.93  $\mu\text{g/L}$  and a median concentration of 0.012  $\mu\text{g/L}$ . The frequent occurrence of these compounds in surface-water samples may warrant consideration for future monitoring and possible consideration by other Federal and State programs.

## Commonly Occurring Anthropogenic Organic Compounds in Groundwater

Ninety-three (about 35 percent) of the 265 AOCs monitored were detected in one or more groundwater samples, and 172 AOCs (about 65 percent) were never detected using an assessment level (appendix 3). Twenty-eight compounds were found to commonly occur in groundwater samples (fig. 7). Using the assessment level of 0.05  $\mu\text{g/L}$ , three compounds were detected in more than 10 percent of samples. Of these three compounds, chloroform was the most commonly occurring compound (23.9 percent) followed by MTBE (12.3 percent) and perchloroethene (PCE; 11.6 percent). Potential sources of chloroform to groundwater include chlorinated water or wastewater that has recharged the aquifer through leaking drinking-water distribution and sewer pipes or from irrigation of athletic fields, lawns, gardens, golf courses, and parks (Ivashenko and Zogorski, 2006; Zogorski and others, 2006); and septic system effluent (DeWalle and others, 1985; Carter and others, 2012). Potential sources of MTBE include leaking storage tanks, urban storm runoff, leaking watercraft tanks, and used motor oils (Zogorski and others, 2006). Perchloroethene is a chlorinated solvent used in commercial

dry cleaning and household degreasers (Zogorski and others, 2006). Chloroform, MTBE, and PCE are among the most commonly occurring compounds found in groundwater in a national ambient resources assessment conducted by the USGS (Zogorski and others, 2006). This may indicate that compounds found to frequently occur in broad-scale resource assessments also may be present in source water. This section focuses on compound occurrence in groundwater. Concentrations are evaluated in more detail in the “Comparison of Surface-Water and Groundwater Occurrence” section.

A wide variety of compounds were detected in groundwater samples. Compounds from 7 of the 13 use groups were found to commonly occur indicating that a wide variety of sources and pathways exist for these compounds to reach these wells. The use group with the largest number of commonly occurring compounds was the herbicides and herbicide degradates group followed by the solvents and disinfection by-products groups (fig. 6).

Nine of the 28 commonly occurring compounds in groundwater were herbicides and herbicide degradates. Their frequency of detection is due, in part, to their widespread use compared to other compounds and may be an artifact of the larger number of herbicides analyzed in samples in comparison to other compounds. Previous studies indicate that herbicide degradates typically occur with their parent compounds at concentrations similar to or greater than concentrations of their parent compounds (Thurman and others, 1992; Kalkhoff and others, 1998; Gilliom and others, 2006). Two degradates of atrazine, 2-hydroxyatrazine and deethylatrazine, are examples of compounds that are detected more frequently than the parent compound (Thurman and others, 1992; Kalkhoff and others, 1998; Gilliom and others, 2006). Atrazine and both degradates were among the most frequently detected herbicides and herbicide degradates, detected in about 3 to 4 percent of the samples at an assessment level of 0.05  $\mu\text{g/L}$ . The degradate 2-hydroxyatrazine was the most frequently detected herbicide degradate and the most frequently detected compound in the herbicides and herbicide degradates use group (detected in 3.9 percent of samples using an assessment level). The degradate 2-hydroxyatrazine was detected in 10.3 percent of samples without an assessment level with concentrations ranging from 0.001 to 0.24  $\mu\text{g/L}$  and a median concentration of 0.03  $\mu\text{g/L}$ . Deethylatrazine was the second most frequently detected herbicide degradate using an assessment level (detected in 3.4 percent of samples). Deethylatrazine was detected in 32.5 percent of samples without an assessment level with concentrations ranging from 0.001 to 0.28  $\mu\text{g/L}$  and a median concentration of 0.01  $\mu\text{g/L}$ , and atrazine was the most frequently detected herbicide (third most frequently detected compound in the herbicide and herbicide degradate use group) using an assessment level, detected in 2.7 percent of samples. Atrazine was detected in 27.8 percent of samples without an assessment level with concentrations ranging from 0.001 to 0.44  $\mu\text{g/L}$  and a median concentration of 0.01  $\mu\text{g/L}$ . The frequency of atrazine occurrence is due, in part, to the widespread use as a weed control on crops and trees.

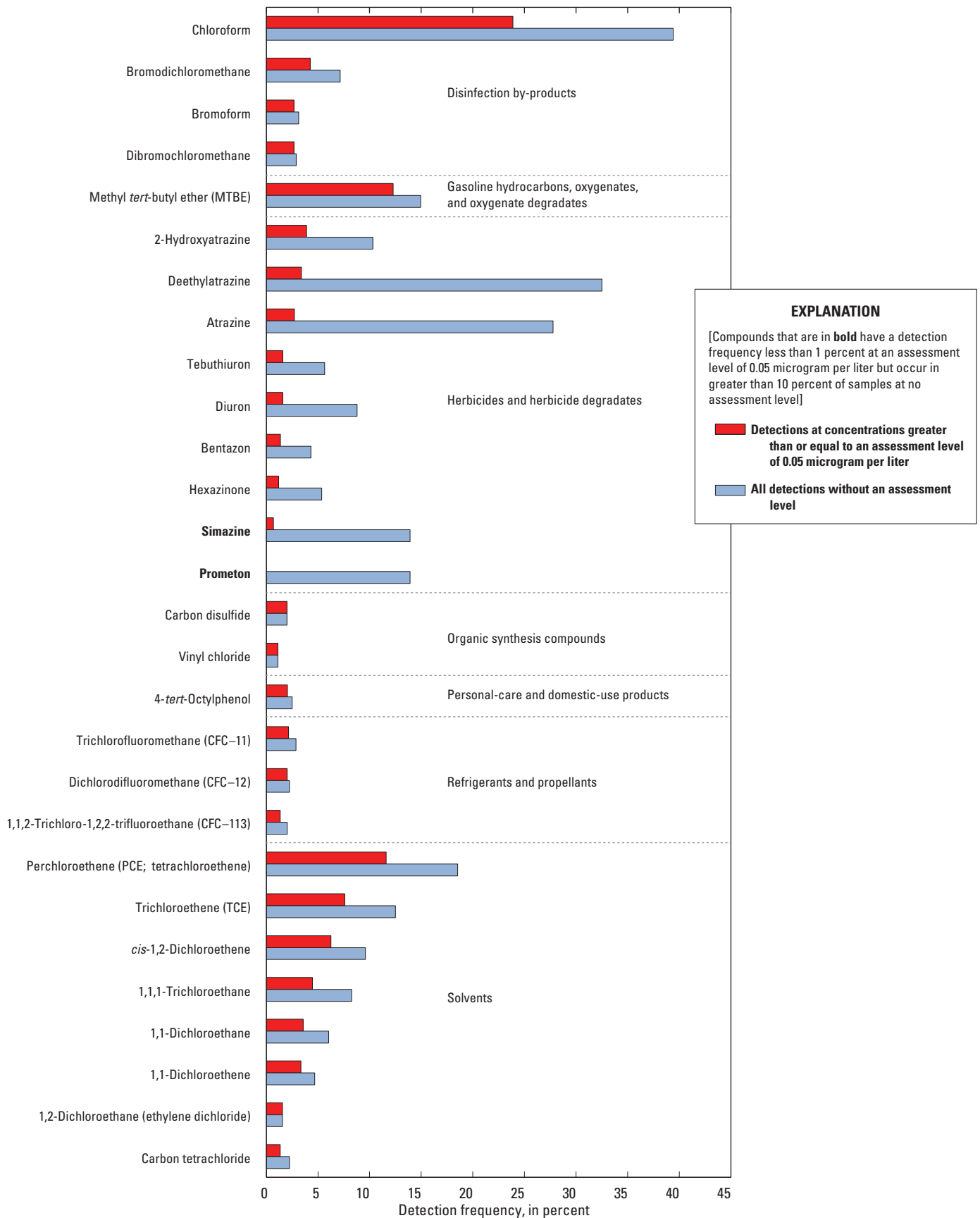


Figure 7. Commonly occurring compounds in source water derived from groundwater.

The U.S. Environmental Protection Agency (2012d) reported that an estimated 75 percent of all field corn acreage grown in the United States is treated with atrazine.

Solvents were the second most commonly occurring use group in groundwater. Their frequent detection is due, in part, to their widespread use in both industry and in household consumer products, such as oven cleaners and household degreasers (U.S. Environmental Protection Agency, 1980; Zogorski and others, 2006). Solvents also are used to decaffeinate coffee and tea and for the extraction of hops (Halogenated Solvents Industry Alliance, 2010). Perchloroethene was the most frequently detected solvent, detected in 11.6 percent of the samples at an assessment level of 0.05 µg/L. Perchloroethene was detected in 18.5 percent of samples without an assessment level with concentrations ranging from 0.01 to 76.8 µg/L and a median concentration of 0.09 µg/L. The solvent, methyl ethyl ketone (MEK), though not one of the commonly occurring compounds, was detected at the highest concentration (2,940 µg/L) of all AOCs, in one groundwater sample (appendix 5). MEK has various industrial uses and primarily is used as a solvent in protective coatings (U.S. Environmental Protection Agency, 1994). Methyl ethyl ketone also is a major component in adhesives, specifically as a component of polyvinyl chloride (PVC) glues. The high concentration of MEK could be attributed to the PVC glues that were used in the plumbing at the wellhead of the supply well sampled. The PVC glues may have contaminated the water at the sampling point, and the high concentration may not represent the concentration of MEK in the aquifer.

Four disinfection by-products commonly occurred in groundwater samples. Using an assessment level of 0.05 µg/L, chloroform was the most frequently detected disinfection by-product (23.9 percent), followed by bromodichloromethane (detected in 4.2 percent), bromoform (detected in 2.7 percent), and dibromochloromethane (detected in 2.7 percent). Chloroform was detected in 39.4 percent of samples without an assessment level with concentrations ranging from 0.009 to 24.7 µg/L and a median concentration of 0.07 µg/L. Bromodichloromethane was detected in 7.1 percent of samples without an assessment level with concentrations ranging from 0.016 to 0.79 µg/L and a median concentration of 0.06 µg/L. Bromoform was detected in 3.1 percent of samples without an assessment level with concentrations ranging from 0.035 to 1.9 µg/L and a median concentration of 0.37 µg/L. Dibromochloromethane was detected in 2.9 percent of samples with concentration ranging from 0.048 to 1.01 µg/L and a median concentration of 0.19 µg/L. Chloroform and the other three disinfection by-products analyzed in samples (bromodichloromethane, bromoform, and dibromochloromethane) commonly are produced during the chlorination of water and wastewater (Ivahnenco and Zogorski 2006). Sources of these disinfection by-products to groundwater can include, in part, municipally supplied chlorinated water to irrigate lawns, golf courses, parks, gardens, and other areas; regulated discharge of chlorinated wastewater to rivers or groundwater recharge facilities; leakage of chlorinated water from swimming pools,

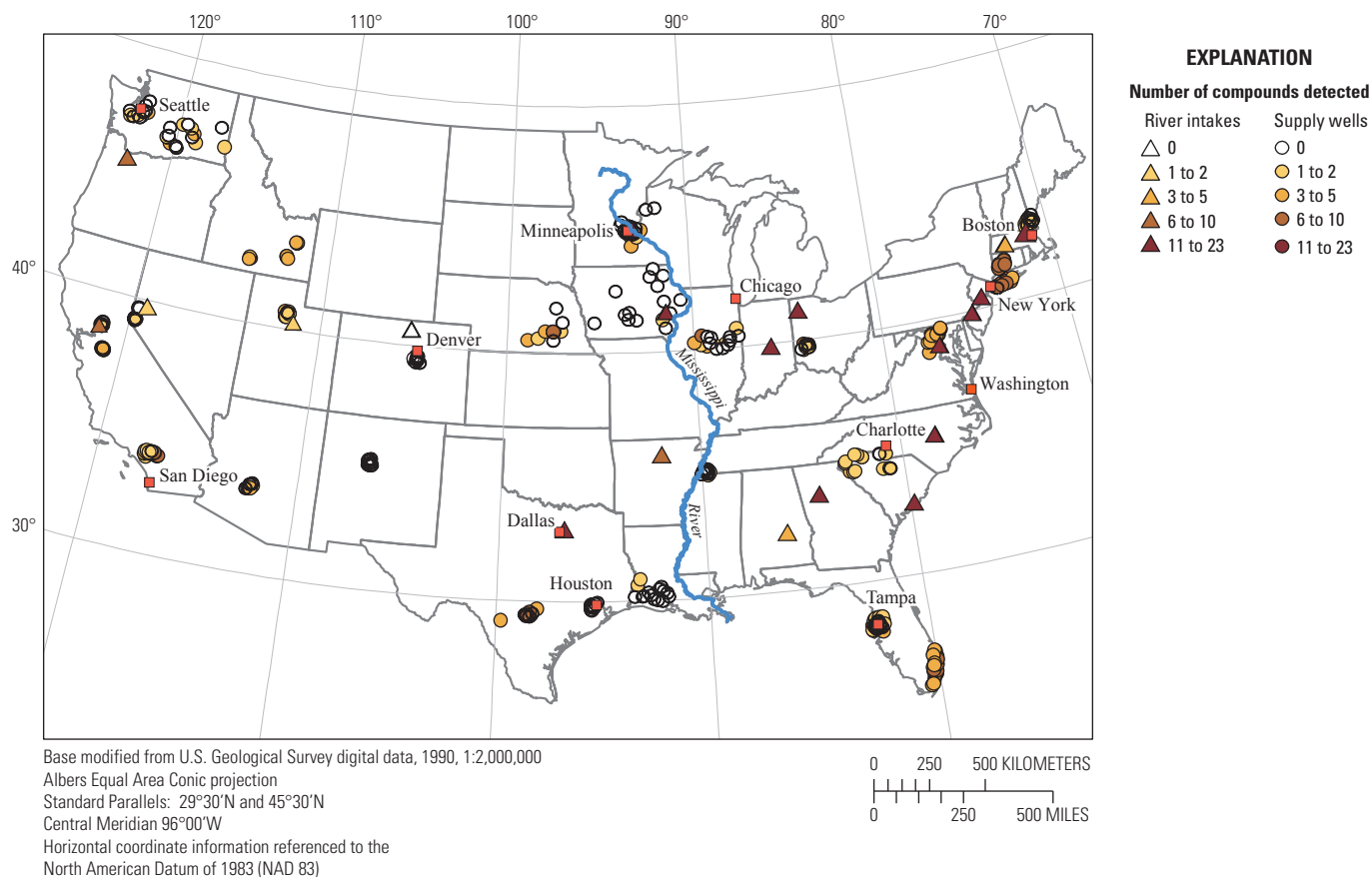
spas, or distribution systems for drinking water or wastewater sewers; domestic well disinfection through chlorination (shock chlorination); laundry wastewater containing bleach; or septic system effluent (Ivahnenco and Zogorski 2006; Carter and others, 2012).

Three of the 28 commonly occurring compounds were on the CCL3: 1,1-dichloroethane, diuron, and MTBE. The compound 1,1-dichloroethane was detected in 6 percent of samples without an assessment level with concentrations ranging from 0.011 to 4.89 µg/L and a median concentration of 0.11 µg/L. Diuron was detected in 8.8 percent of samples without an assessment level with concentrations ranging from 0.003 to 0.17 µg/L and a median concentration of 0.021 µg/L. Methyl *tert*-butyl ether was detected in 15 percent of samples without an assessment level with concentrations ranging from 0.027 to 2.96 µg/L and a median concentration of 0.14 µg/L. The frequent occurrence of these compounds in groundwater samples may warrant consideration for future monitoring and possible consideration by other Federal and State programs.

## Comparison of Surface Water and Groundwater Occurrence

Many factors affect the occurrence of the AOCs monitored in both surface water and groundwater used as sources of drinking water. To better understand the spatial occurrence of compounds in source waters, a geographic distribution of the number of commonly detected compounds detected in samples without an assessment level is shown in figure 8. In general, 11 or more compounds were detected in samples collected from rivers in the more populated areas located east of the Mississippi River. Similarly, three or more compounds were detected in samples collected from supply wells in these same areas of the country. Fewer compounds were detected in samples collected from rivers and supply wells west of the Mississippi River than east of the Mississippi River. None of the samples from one surface-water site (Cache la Poudre River) had any detections of AOCs. Samples collected from most of the supply wells in the Midwest (that is, Iowa, Illinois, and Wisconsin) and in Tennessee and Louisiana had no compounds detected. Spatially evaluating the number of compounds detected in surface water and groundwater illustrates how possible sources of these compounds and factors such as population can affect these two source water types.

Although most comparisons within this study primarily focus on the most commonly occurring compounds, a brief overview of all compounds monitored is warranted. Of the 265 AOCs monitored at all sites, 158 compounds were detected in one or more surface-water samples, representing 12 of the 13 use groups (appendix 2). The three compounds in the refrigerants and propellants group were not detected in surface-water samples. A total of 156 AOCs were detected in one or more groundwater samples, which included all 13 use groups (appendix 3). About one-half the 265 compounds monitored (122) were detected in one or more samples collected



**Figure 8.** Geographic distribution of the number of commonly detected compounds without an assessment level in surface-water and groundwater samples collected from 20 river intakes and 448 supply wells during 2002–10.

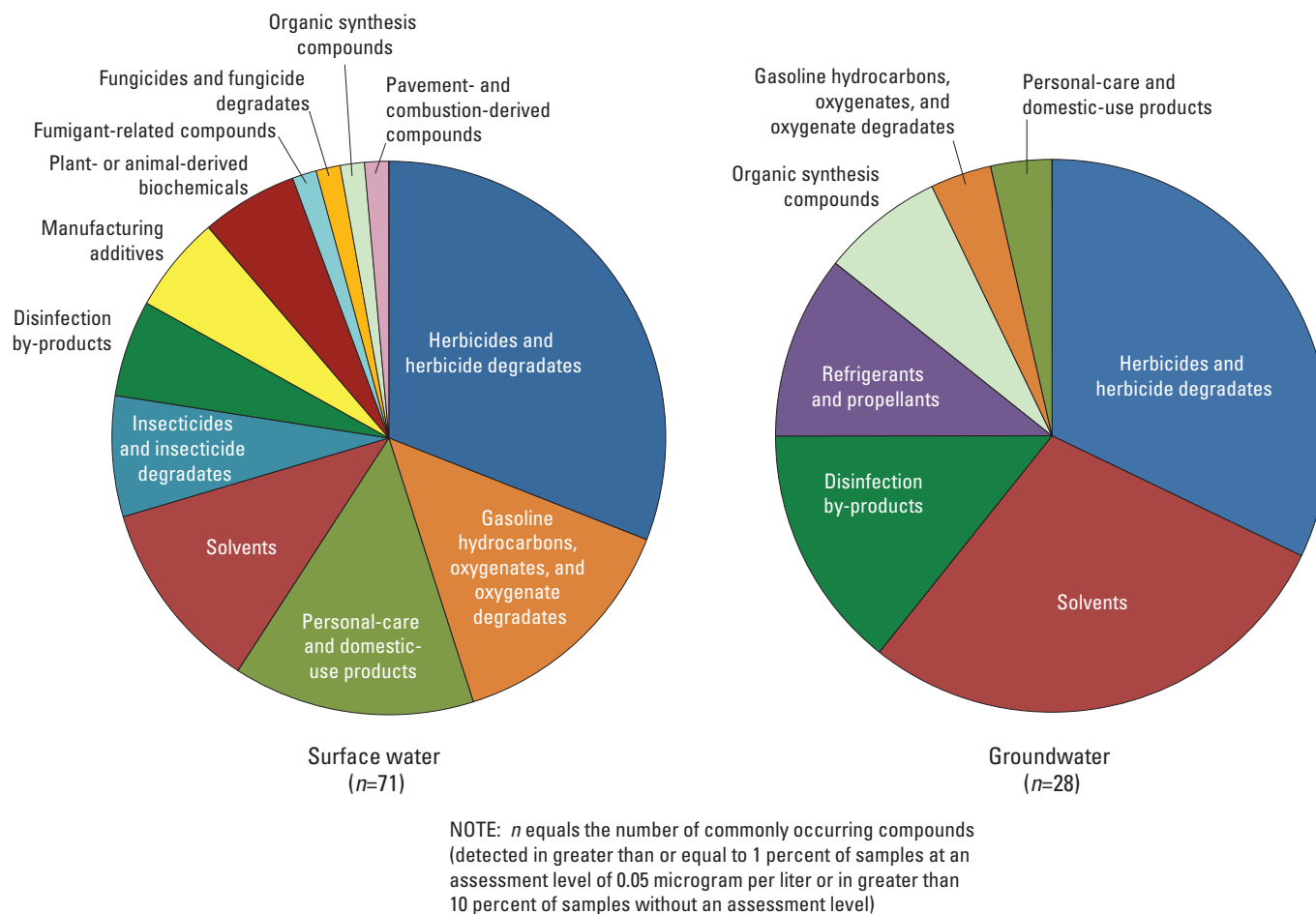
from both surface water and groundwater. About 28 percent of the compounds monitored (73 of 265 AOCs) were never detected in either type of water samples. About 14 percent of the compounds monitored (36 AOCs) were detected only in surface-water samples, whereas about 13 percent (34) were detected only in groundwater samples. Of the 68 herbicide and herbicide degradates monitored at all sites, 54 percent (37) were detected in one or more samples of both water types. Most (19 of 27) of the gasoline hydrocarbons, oxygenates, and oxygenate degradates that were monitored were detected in one or more samples of both water types. All 4 disinfection by-products and all 5 plant- or animal-derived biochemicals were detected in both water types. The occurrence of compounds with varying uses in both water types further indicates that these compounds have a variety of sources and pathways to enter water supplies.

Comparisons of the occurrence of the most commonly occurring compounds in surface water and groundwater were made using no assessment level. A common assessment level is not used when comparing river and groundwater results because comparisons of the same compound and use group were made between water types. Therefore, the analytical sensitivity that would otherwise warrant an assessment level when comparing between compounds or use groups is no longer necessary.

The 71 and 28 commonly occurring compounds identified in surface water and groundwater, respectively (figs. 6 and 7), were used as the primary basis for comparison between surface water and groundwater. Combining these two lists resulted in 84 compounds used for comparisons between the two water types. It is important to note that the 84 compounds were defined as commonly occurring in one or both water types.

A more diverse suite of commonly occurring compounds was detected in surface water than groundwater (fig. 9). The occurrence of compounds from a variety of use groups indicates that a wide variety of sources and pathways exist for these compounds to reach both types of source water. Herbicides and herbicide degradates were the most commonly detected group of compounds in surface water and groundwater. Beyond that similarity, a different chemical signature was observed between the two water types. The gasoline hydrocarbons, oxygenate, and oxygenate degradates group and the personal-care and domestic-use products group were the next most frequently detected use groups in surface-water samples. Solvents were the second most frequently detected group in groundwater, followed by disinfection by-products, and refrigerants and propellants.

Of the 84 commonly occurring compounds, 65 compounds were detected in one or more samples of both surface



**Figure 9.** Characterization of use groups for commonly occurring compounds in surface water and groundwater.

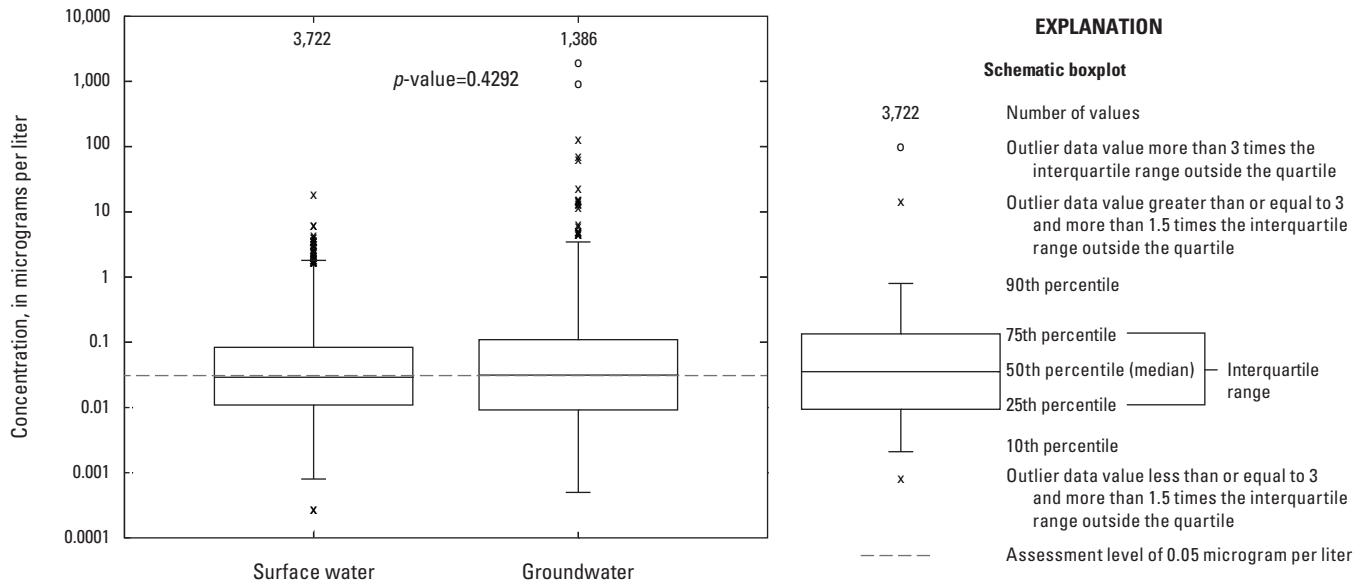
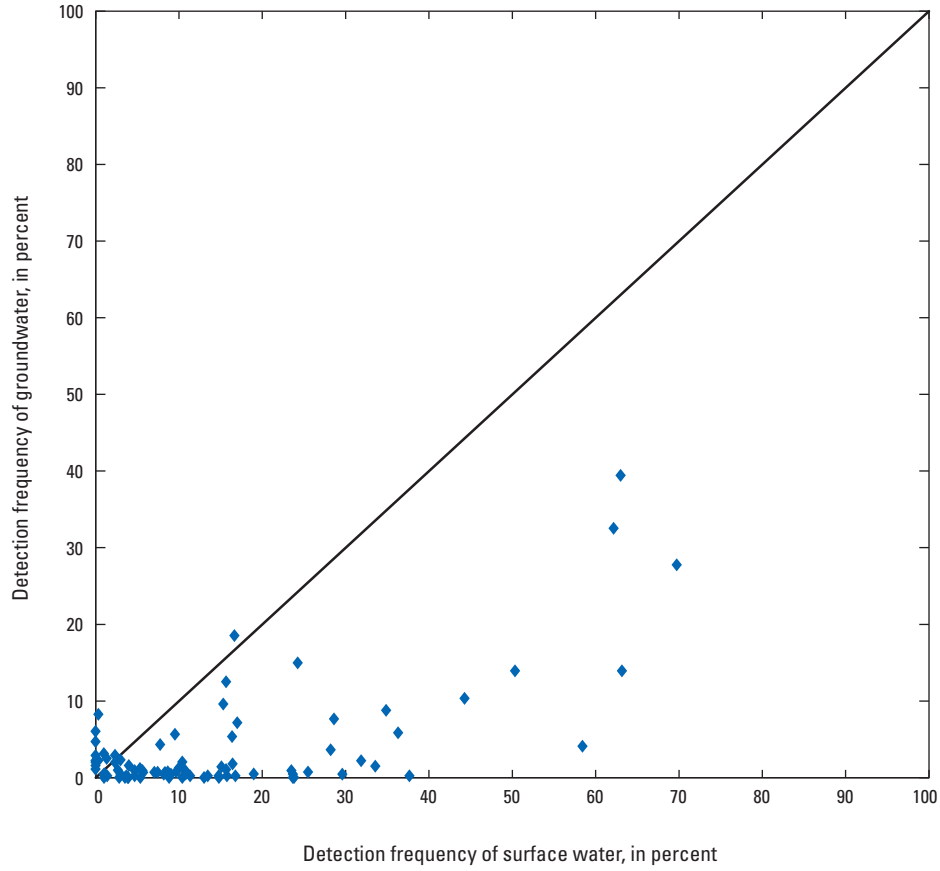
water and groundwater. For commonly occurring compounds detected in both water types, the detection frequency was higher for surface-water samples than groundwater samples; however, concentrations were not significantly different (rank-sum test;  $p$ -value=0.4292) (fig. 10). When detected, concentrations of the 84 compounds ranged from 0.0003 to 20.1  $\mu\text{g/L}$  in surface-water samples and from 0.0005 to 2,090  $\mu\text{g/L}$  in groundwater samples. The median concentrations were 0.029  $\mu\text{g/L}$  and 0.032  $\mu\text{g/L}$  for surface water and groundwater, respectively. Concentrations for a small subset of detections were greater than 1  $\mu\text{g/L}$  (2 and 5 percent in surface water and groundwater, respectively). Most of the concentrations (63 and 61 percent in surface water and groundwater, respectively) were less than 0.05  $\mu\text{g/L}$ . This highlights the significance of low-level analytical and field processing methods to gain a better understanding of the occurrence of these types of compounds in source water.

Analysis of individual use groups for the 65 commonly occurring compounds in both surface water and groundwater indicated different patterns in concentrations between surface water and groundwater. Compounds in the herbicides and herbicide degradates group and the personal-care and domestic-use products group were detected more frequently in surface

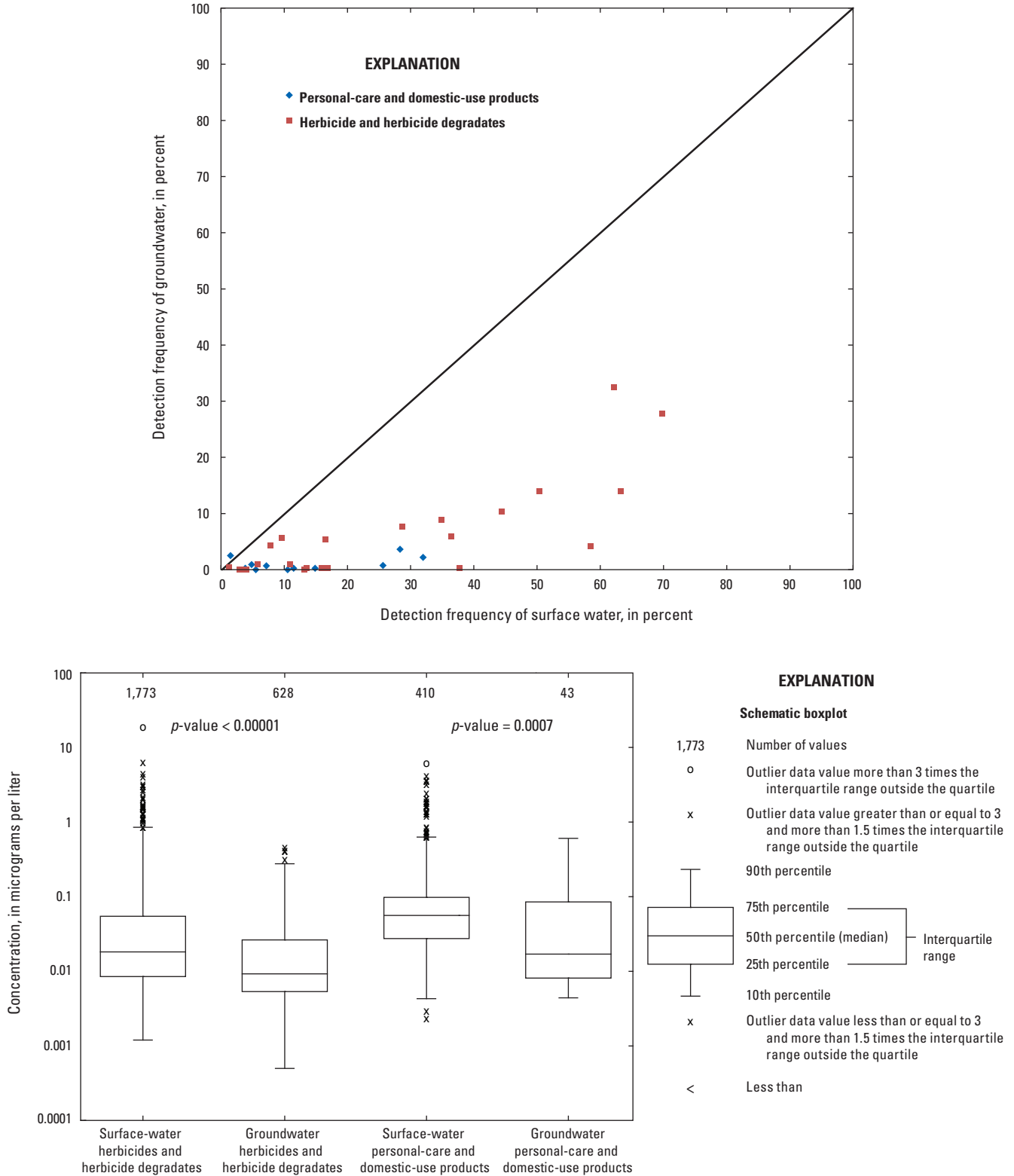
water than groundwater, and concentrations of compounds in both use groups were significantly greater in surface water than in groundwater (fig. 11). Some disinfection by-products and solvents were detected more frequently in surface water, whereas others were detected more frequently in groundwater; however, concentrations were significantly larger ( $p$ -values less than 0.05) for both groups of compounds in groundwater (fig. 12). These findings indicate that although compounds generally may be more frequently detected in surface water than groundwater and have similar concentrations, both detection frequency and concentration may be larger in either water type depending on the compound's primary use and physical/chemical properties. For example, solvents may occur more frequently at larger concentrations in groundwater than surface water because of their volatility. Similarly, personal-care and domestic-use products may occur more frequently at higher concentrations in surface water because of their introduction to rivers from wastewater effluent discharges or other sources. This highlights the importance of understanding the sources and pathways for a compound to enter source water as well as the compound's physical and chemical properties.

Four compounds in surface water and three compounds in groundwater were commonly occurring and are included

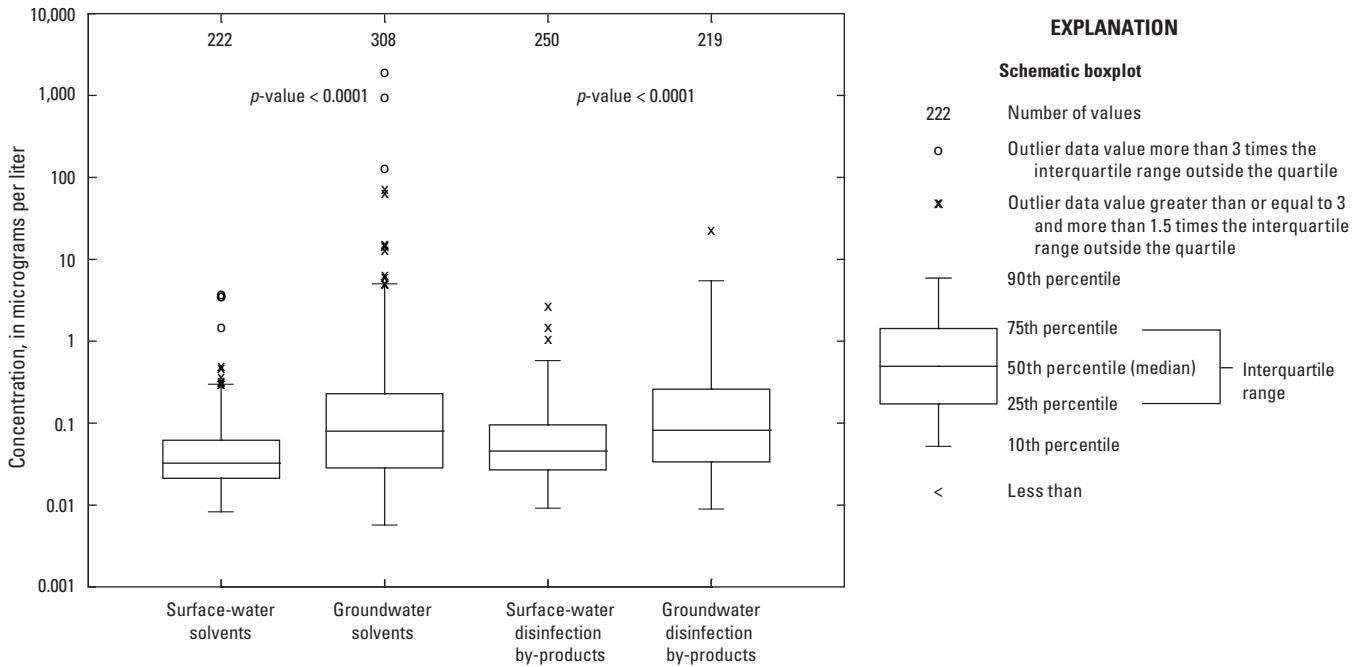
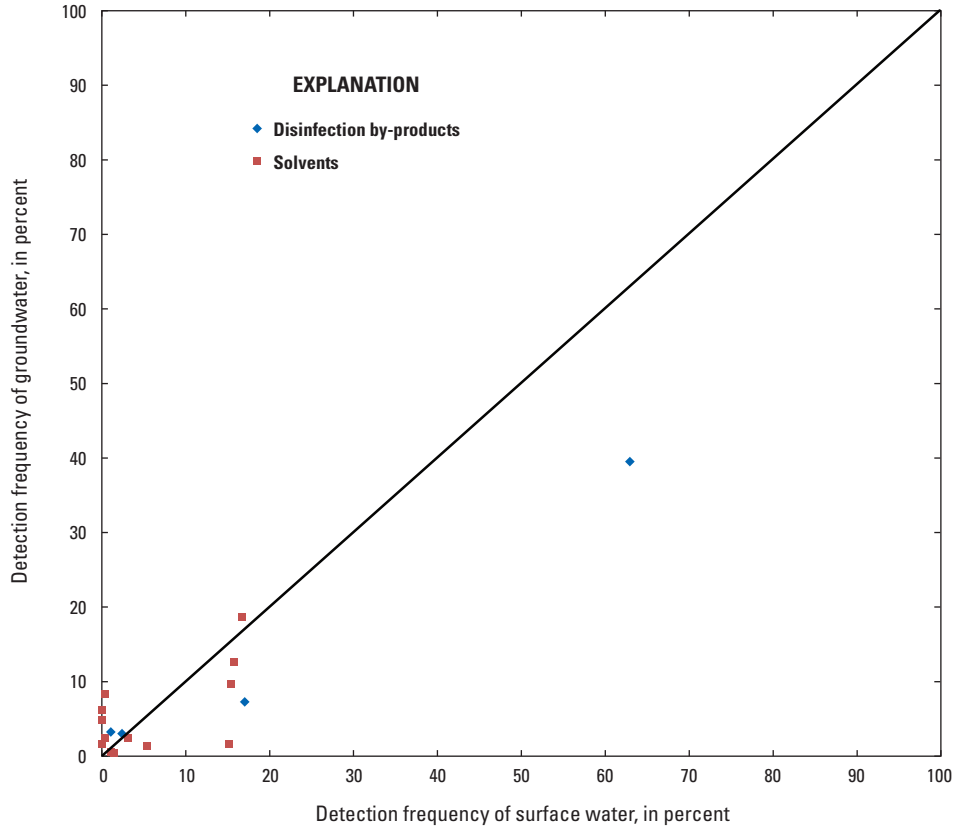




**Figure 10.** Detection frequency and quantified concentrations of 65 commonly occurring compounds in both surface water and groundwater using no assessment level.



**Figure 11.** Detection frequency and quantified concentrations of commonly occurring herbicide and herbicide degradates and personal-care and domestic-use products in surface water and groundwater.



**Figure 12.** Detection frequency and quantified concentrations of commonly occurring disinfection by-products and solvents in surface water and groundwater.

on the CCL3 list. Two of these compounds on the CCL3 were found to occur commonly, at no assessment level, in samples of both water types: MTBE and diuron. The gasoline oxygenate MTBE was detected more frequently in surface water (24.3 percent) than in groundwater (15 percent). Similarly, the herbicide diuron was detected more frequently in surface water (34.9 percent) than in groundwater (8.8 percent). The frequent occurrence at no assessment level of these two compounds in surface-water and groundwater samples may warrant consideration for future monitoring and possible consideration by other Federal and State programs.

## Comparison of Results to Human-Health Benchmarks in Surface Water and Groundwater

Human-health benchmarks were available for more than one-half the compounds (160 of the 265) that were monitored at all sites. Of the most commonly occurring compounds in surface water, 58 percent (41 of 71 AOCs) have a human-health benchmark to which concentrations can be compared. Of the 71 compounds that are commonly occurring in surface-water samples, 19 have MCLs and 22 have HBSLs. Five compounds had concentrations greater than or within one-tenth of a benchmark: 4 herbicides and herbicide degradates and 1 insecticide (fig. 13A). Two of the five compounds (simazine and atrazine) have MCLs, and acetochlor, diuron, and fipronil have HBSLs. Atrazine was the only compound to have concentrations greater than the benchmark. Atrazine concentrations were greater than the MCL in three samples, all of which were collected from the same site (White River in Indiana). Although only 3 samples had concentrations greater than the MCL, atrazine had many (35) detections within one-tenth of the benchmark. Fipronil and simazine had 18 and 14 detections, respectively, within one-tenth of the benchmark. None of the five compounds had an annual mean concentration within one-tenth of the benchmark; the median concentration of the annual mean concentrations for each site is shown on figure 13.

Of the 28 most commonly occurring compounds in groundwater, 24 compounds have a human-health benchmark to which concentrations can be compared: 14 compounds have MCLs and 10 compounds have HBSLs. Nine of the most commonly occurring compounds had concentrations greater than or within one-tenth of a benchmark: 1 disinfection by-product (chloroform), 1 herbicide (atrazine), 1 organic synthesis compound (vinyl chloride), and 6 solvents (fig. 13B). All nine compounds—chloroform, atrazine, vinyl chloride, 1,1-dichloroethene, 1,2-dichloroethane, carbon tetrachloride, *cis*-1,2-dichloroethene, perchloroethene (PCE), and trichloroethene (TCE)—have MCLs to which concentrations can be compared. Perchloroethene and TCE were the only compounds with concentrations greater than the benchmark. Concentrations of PCE were greater than the MCL in 3 samples and within one-tenth of the benchmark in 9 samples. Concentrations of TCE were greater than the MCL in 3 samples and

within one-tenth of the benchmark in 5 samples. Concentrations of 1,1-dichloroethene in four samples and concentrations of vinyl chloride in three samples were within one-tenth of their respective benchmarks. Concentrations of atrazine in 2 samples and concentrations of chloroform, 1,2-dichloroethane, carbon tetrachloride, and *cis*-1,2-dichloroethene in 1 sample were within one-tenth of their respective benchmarks.

Three compounds detected in surface-water samples that were not commonly occurring—iprodione, molinate, and dieldrin—had concentrations within one-tenth of a human-health benchmark (appendix 4). Dieldrin was the only compound with a median concentration of the annual mean concentrations that was greater than its human-health benchmark when compared to the low end ( $10^{-6}$ ) of the HBSL range ( $10^{-6}$  to  $10^{-4}$  cancer risk level; Toccalino and others, 2008). However, dieldrin was only detected in 2 of 306 samples, and one-quarter of the LRL (which was used in calculating the median of the annual mean concentration for nondetected concentrations) was larger than the low end of the HBSL. As such, the median of the annual mean concentration for dieldrin may be overestimated. Because of this, future monitoring for dieldrin may need to consider the use of a lower-level analytical method.

In groundwater, some compounds that were not commonly occurring had concentrations greater than a human-health benchmark value including 1,2-dibromo-3-chloropropane; 1,2-dibromoethane; dieldrin (low end of HBSL range); and acrylonitrile (low end of HBSL range) (appendix 5). Other compounds that did not exceed a benchmark value but that had concentrations within one-tenth of a benchmark include benzene, alachlor, and methyl ethyl ketone (MEK) (appendix 5).

Rivers had almost one-half as many commonly occurring compounds (5) within at least one-tenth of a benchmark in comparison to groundwater (9) (fig. 13). However, the number of times these compounds exceed one-tenth of a benchmark was about twice as often as in groundwater. In general, concentrations in groundwater are thought to be relatively stable for longer periods of time in comparison to temporal concentration fluctuations in rivers (Schroeder 2003; Bender and others, 2009). As such, the common occurrence (more than 10 percent) in either water type is considered to be equally important.

Of the 265 compounds monitored, 105 compounds do not have a human-health benchmark (an MCL for regulated compounds or an HBSL for unregulated compounds) to compare concentrations with. Of these 105 compounds, 49 were detected in one or more samples of both types of source water. With respect to the 84 commonly occurring compounds in surface water, groundwater, or both, about two-thirds (52 of the 84) have a human-health benchmark, whereas 32 do not have a human-health benchmark. Of these 32, 17 were detected in 10 percent or more source-water samples from either water type (table 6). For these 17 compounds, their frequent occurrence in surface water or groundwater, or both, directly supplying CWSs may warrant the development of appropriate toxicity information that would allow the ability to calculate an HBSL value (or range in values) to which

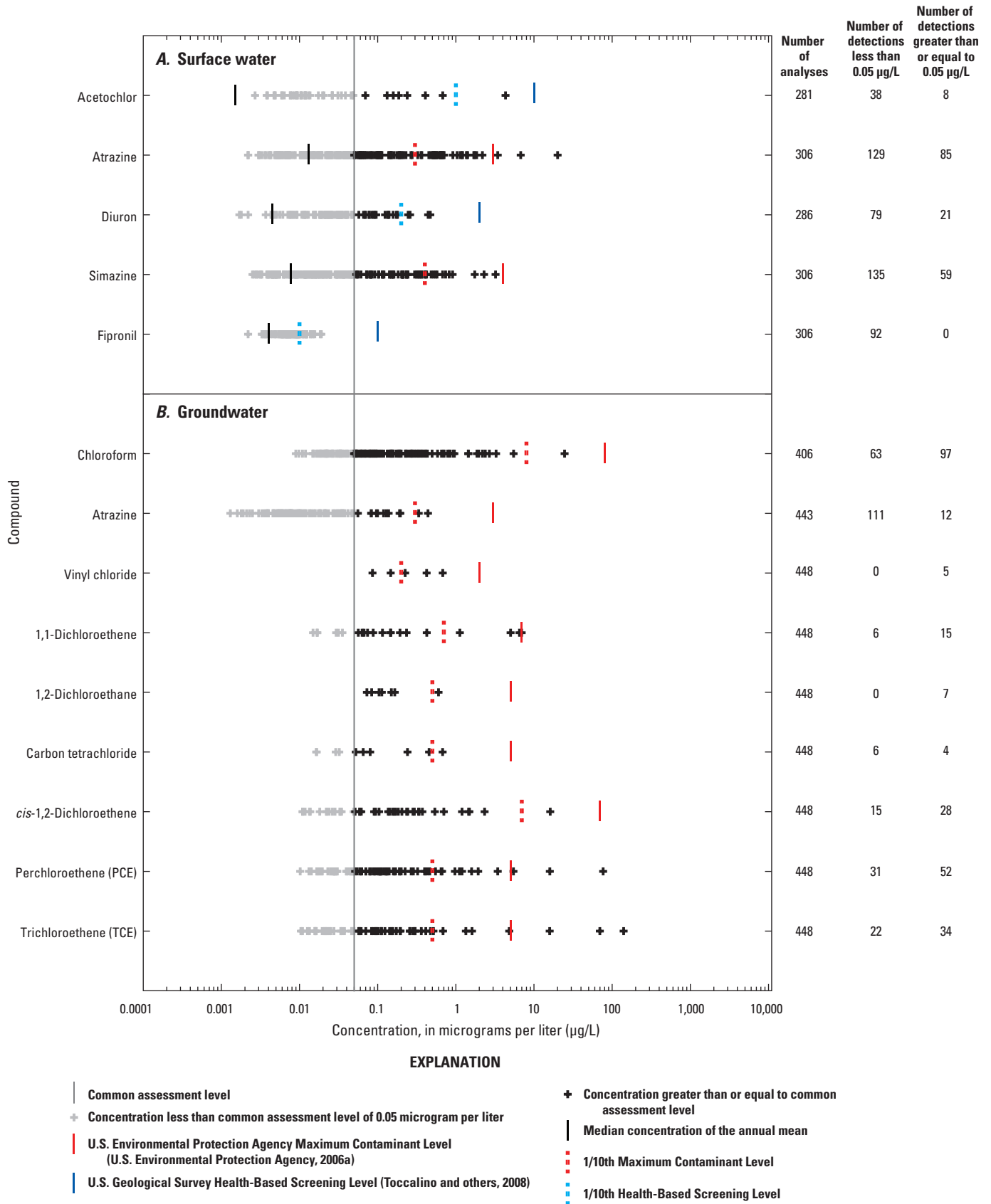


Figure 13. Commonly occurring compounds with concentrations that exceeded or were within one-tenth of a benchmark in A, surface water and B, groundwater.

**Table 6.** List of compounds without a human-health benchmark that were detected in greater than 10 percent of samples from surface water or groundwater, or both (no assessment level).

[Shaded rows indicate compounds on U.S. Food and Drug Administration Generally Recognized As Safe list (U.S. Department of Health and Human Services, 2011). CASRN, Chemical Abstract Services Registry Number; --, no information available]

Compound name	CASRN <sup>a</sup>	Detection frequency (percent)	
		Surface water	Groundwater
Deethylatrazine	6190–65–4	62	33
Methyl <i>tert</i> -butyl ether (MTBE) <sup>b</sup>	1634–04–4	24	15
3,4-Dichloroaniline	95–76–1	36	6
Hexahydrohexamethyl-cyclopentabenzopyran (HHCB)	1222–05–5	32	2
Deisopropylatrazine	1007–28–9	29	8
Acetyl hexamethyl tetrahydronaphthalene (AHTN)	21145–77–7	26	1
Tri(2-butoxyethyl)phosphate	78–51–3	24	0
Desulfinylfipronil	--	24	0.4
Tris(dichlorisopropyl) phosphate	13674–87–8	23	1
Cholesterol	57–88–5	19	0.5
Fipronil sulfide	120067–83–6	16	2
<i>p</i> -Cresol	106–44–5	15	1
Camphor	76–22–2	11	0.2
Nonylphenol, diethoxy- (total)	26027–38–2	10	0
1,2,4-Trimethylbenzene	95–63–6	10	1
Caffeine	58–08–2	28	4
Triethyl citrate	77–93–0	15	0.2

<sup>a</sup>This report contains Chemical Abstracts Service Registry Numbers (CASRN)<sup>®</sup>, which is a Registered Trademark of the American Chemical Society. The CASRN online database provides the latest registry number information: <http://www.cas.org/>. Chemical Abstracts Service recommends the verification of the CASRNs through CAS Client Services<sup>SM</sup>.

<sup>b</sup>Although no human-health benchmark (MCL or HBSL) has been developed for MTBE, the U.S. Environmental Protection Agency has issued a drinking water advisory of 20–40 micrograms per liter for MTBE to avert unpleasant taste and odor effects (U.S. Environmental Protection Agency, 1997).

concentration data can be compared. Lacking this information, it is not possible to interpret results for these compounds in a human-health context.

Two compounds without a human-health benchmark—deethylatrazine and MTBE—were found to occur in more than 10 percent of samples in both water types and may warrant priority development of HSBLs. Deethylatrazine was the most commonly detected compound without a human-health benchmark in surface water (62 percent) and groundwater (33 percent). Methyl *tert*-butyl ether was detected in 24 and 15 percent of surface-water and groundwater samples, respectively. Although no human-health benchmark (MCL or HBSL) has been developed for MTBE, the U.S. Environmental Protection Agency has issued a drinking-water advisory of 20–40 micrograms per liter for MTBE to avert unpleasant taste and odor effects (U.S. Environmental Protection Agency, 1997). The remaining 15 compounds without human-health benchmarks only occurred in more than 10 percent of surface-water samples (table 5). Two of these compounds—triethyl citrate and caffeine—may not warrant the development of a

human-health benchmark because they are included on the U.S. Food and Drug Administration's Generally Recognized As Safe (GRAS) list (U.S. Department of Health and Human Services, 2011).

## Factors Affecting the Occurrence of Compounds in Surface Water and Groundwater

Most of the AOCs monitored in this study are used in urban or agricultural settings, or both. Some compounds enter source waters after application on the land surface, such as herbicides and insecticides that are used in both types of settings, but are used more systematically in agricultural settings. Transport to surface water occurs with rainfall and runoff and also from groundwater discharge that has been affected by infiltration of herbicides and insecticides or other AOCs with recharge. Sources of other groups of compounds, such as solvents and organic synthesis compounds, primarily are from accidental releases or historical disposal in landfills (Zogorski and others, 2006). A source of personal-care and domestic use

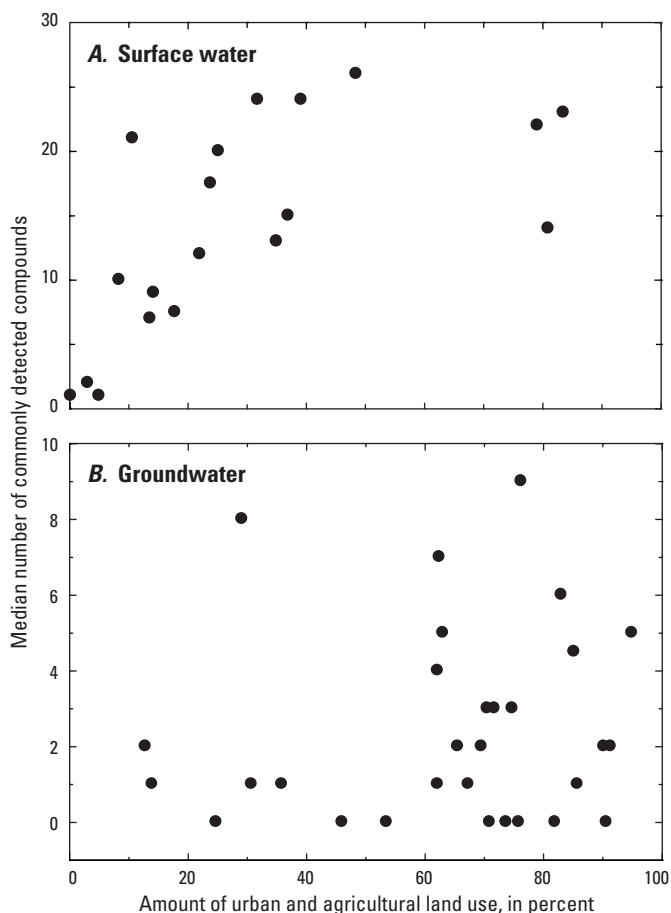
compounds is the discharge of treated wastewater to streams (Kingsbury and others, 2008).

In surface water, the amount of urban and agricultural land in the watershed was related to the occurrence of commonly occurring compounds in source water (fig. 14A). The number of commonly occurring compounds detected in surface-water samples generally increased as the amount of urban and agricultural land increased (fig. 14A). Most surface-water sites had a median of 5 or more compounds detected in samples with a maximum of 26 compounds. Samples from sites for which approximately 25 percent or more of the watershed had urban and agricultural land use (about one-half of the sites) typically had 14 or more compounds detected. Conversely, only 1 or 2 compounds were detected in samples from sites with 5 percent or less urban and agricultural land use.

The herbicides and herbicide degradates group were the most commonly detected use group in surface water. With the exception of the Cashe la Poudre site, at least one herbicide was detected at each site, and the number of samples with detections and the summed concentrations of herbicides generally increased with the amount of agricultural land use in the watershed (fig. 15). For example, sites with larger percentages (that is, greater than 10 percent) of agricultural land were more likely to have samples with total herbicide concentrations greater than 1  $\mu\text{g/L}$ . The summed concentrations of herbicides for samples from sites with less than 10 percent agricultural land use almost always were less than 0.1  $\mu\text{g/L}$ .

Atrazine and simazine were two of the most commonly occurring herbicides, but their occurrence relative to the amount of agricultural land in the watershed differed. Both atrazine and simazine have agricultural and nonagricultural uses, but simazine has substantial nonagricultural use (Gilliom and others, 2006; Kingsbury and others, 2008). The association between simazine occurrence, in particular the concentrations at which it was detected, and the amount of agricultural land in the watershed, is much less evident than that of atrazine (fig. 15).

In general, some of the more commonly detected compounds in rivers have chemical signatures indicating municipal or industrial wastewater discharge. Examples of some of the more frequently occurring compounds in rivers include hexahydrohexamethylcyclopentabenzopyran (HHCb), chloroform, tris(dichlorisopropyl) phosphate, cholesterol, and 3-*beta*-coprostanol. Results from this study are consistent with other national studies that have linked these compounds to wastewater discharges (Kolpin and others, 2002; Kingsbury and others, 2008). For example, the fragrance compound HHCb was the most frequently occurring compound in rivers at an assessment level of 0.05  $\mu\text{g/L}$ . Hexahydrohexamethylcyclopentabenzopyran commonly is used in detergents and other personal-care products and has been found in both influent and effluent of wastewater-treatment plants in the United States and Europe (Bester, 2004; Phillips and others, 2005). The disinfection by-product, chloroform, was the second most commonly detected compound in rivers and may be present in treated wastewater because of the household use of bleach



**Figure 14.** Relation between median number of commonly occurring compounds detected and the amount of urban and agricultural land use in the watershed or contributing area without an assessment level at A, surface-water sites and B, groundwater studies.

as well as the disinfection of wastewater during the treatment process (Ivahnenco and Barbash, 2004; Zogorski and others, 2006). Other possible sources of chloroform include artificial recharge of wastewater, its use as a refrigerant for home air conditioners and large commercial freezers, and its use in reagents, extraction solvents, fumigants, insecticides, and as a precursor for dyes and pesticides (Budavari, 1989; Mannsville Chemical Products Corporation, 1999; Lucius and others, 1992; Agency for Toxic Substance and Disease Registry, 1997; Zogorski and others, 2006). The manufacturing additive tris(dichlorisopropyl)phosphate and the biochemicals cholesterol and 3-*beta*-coprostanol were detected in 13, 19, and 9 percent of samples, respectively, with an assessment level of 0.05  $\mu\text{g/L}$ . These three compounds were detected in a national reconnaissance of emerging compounds in rivers that receive a substantial amount of municipal, industrial, or agricultural wastewater discharge (Kolpin and others, 2002; Kingsbury and others, 2008). The occurrence of these compounds in rivers that receive major wastewater discharge is consistent with several studies that indicate organic compounds, such as

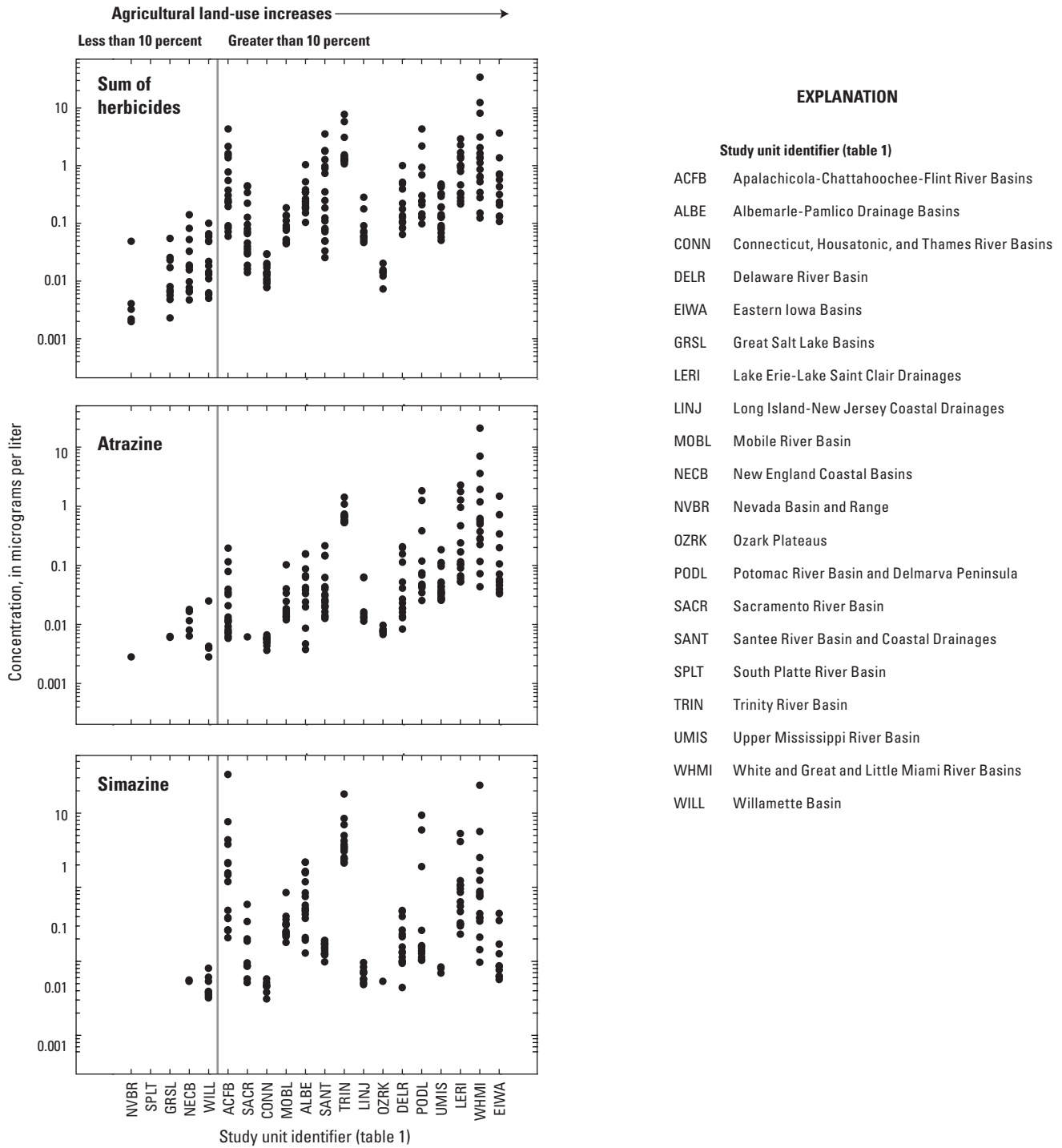


Figure 15. Concentrations of herbicides detected without an assessment level in surface-water samples collected from rivers.



manufacturing additives or animal biochemical compounds, are not removed during the wastewater-treatment process and are detected in the receiving rivers (Halling-Sørensen and others, 1998; Kolpin and others, 2002; Stackelberg and others, 2004; Kingsbury and others, 2008).

In groundwater, the more important factors affecting the occurrence of AOCs include the use of a compound in the contributing area, recharge, and aquifer rock type. Hopple and others (2009) used a subset of the data presented in this report to provide additional information on factors that affect the occurrence of compounds in groundwater. A generalized characterization of the occurrence of commonly detected compounds with respect to factors such as principal aquifer type and the use of compounds in a contributing area will help to put the results into context and explain some of the differences in the occurrence of compounds.

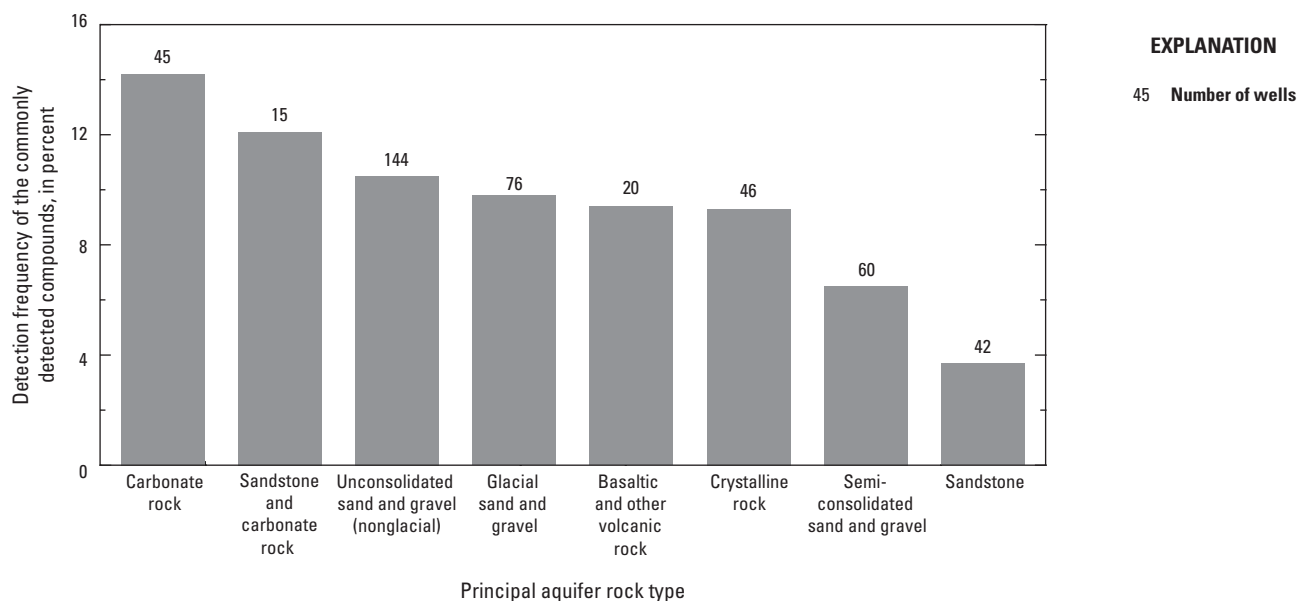
Compounds were found to occur most frequently in samples from wells in carbonate rock types, which were predominantly located in the northeastern part of the country, whereas sandstone aquifers had the lowest detection frequency among the principal aquifer rock types (fig. 16). In general, Hopple and others (2009) found that detection frequencies did not change substantially within a particular lithological group. However, additional factors such as the presence of confining units, well capacity, land use, population density, and the presence of sources of these compounds likely are important factors affecting the occurrence of these compounds.

Determining the land use in the watershed area of a river is relatively straightforward, but is much less so for determining the land use in the contributing area for supply wells. The contributing areas for wells can be approximated with a

groundwater-flow model, but models typically are not readily available for most wells. In this study, land use in a 500-m buffer area around the wells was characterized and assumed to be representative of the land use for the actual contributing areas for the supply wells. This assumption likely is less valid as well depth and pumping capacity increase, but this approach provides an estimate and a framework within which results can be compared among groundwater sites.

Similar to the results for river sites, the number of commonly occurring compounds detected in samples from the supply wells generally increased as the amount of urban and agricultural land near the wells increased (fig. 14B). Most sites with less than 50 percent of these land uses in the contributing areas of the supply wells had detections of two or fewer compounds. For wells where urban and agricultural land use was greater than 50 percent in the contributing area, the median number of compounds detected often was two or more.

In surface water and groundwater, most of the organic compounds monitored in this study are used in urban or agricultural settings, or both. Some compounds end up in source waters after application on the land surface, such as herbicides and insecticides that are used in both types of settings, but are used more systematically in agricultural settings. To put results from this study into context with the national distribution of rivers and supply wells used by CWS, the river and supply-well sites sampled for this study were grouped into the respective national population of land-use quartiles (table 7). The increase in detection frequency with increasing urban and agricultural land use was more evident for samples from rivers than from supply wells (fig. 17). For rivers, the median detection frequency increased for each quartile, with more



**Figure 16.** Detection frequencies without an assessment level of commonly detected compounds by principal aquifer rock type for samples from 448 supply wells collected during 2002–09.

**Table 7.** Number of study sites sampled within land-use quartiles for 2,016 river intakes and 112,099 supply wells considered to represent the national distribution of river intakes and supply wells, respectively, supplying community water systems.[≤, less than or equal to; >, greater than; *n*, number of study locations sampled within this quartile]

Category	Quartile			
	1 ≤25 percent	2 >25–50 percent	3 >50–75 percent	4 >75 percent
Rivers ( <i>n</i> =20)				
Agricultural land use (percent)	0–0.03 ( <i>n</i> =1)	0.04–9 ( <i>n</i> =4)	9.1–27.2 ( <i>n</i> =9)	27.3–94.7 ( <i>n</i> =6)
Undeveloped land use (percent)	0–61.6 ( <i>n</i> =8)	61.7–82.8 ( <i>n</i> =6)	82.9–96.7 ( <i>n</i> =5)	96.8–100 ( <i>n</i> =1)
Urban land use (percent)	0–1.6 ( <i>n</i> =1)	1.7–4.9 ( <i>n</i> =5)	5–8.1 ( <i>n</i> =4)	8.2–86.2 ( <i>n</i> =10)
Urban and agricultural land use (percent)	0–3.1 ( <i>n</i> =1)	3.2–17 ( <i>n</i> =5)	17.1–38.2 ( <i>n</i> =6)	38.3–100 ( <i>n</i> =8)
Population density (people per square kilometer)	0–2.5 ( <i>n</i> =1)	2.6–13.8 ( <i>n</i> =1)	13.9–37.2 ( <i>n</i> =8)	37.3–3.49x10 <sup>9</sup> ( <i>n</i> =10)
Supply wells ( <i>n</i> =448)				
Agricultural land use (percent)	0–0 ( <i>n</i> =272)	0–5.5 ( <i>n</i> =51)	5.6–31.2 ( <i>n</i> =83)	31.3–100 ( <i>n</i> =42)
Undeveloped land use (percent)	0–26 ( <i>n</i> =179)	26.1–54.2 ( <i>n</i> =130)	54.3–81.2 ( <i>n</i> =79)	81.3–100 ( <i>n</i> =60)
Urban land use (percent)	0–3.5 ( <i>n</i> =39)	3.6–16.7 ( <i>n</i> =54)	16.8–45.3 ( <i>n</i> =102)	45.4–100 ( <i>n</i> =253)
Urban and agricultural land use (percent)	0–18.6 ( <i>n</i> =60)	18.7–45.6 ( <i>n</i> =79)	45.7–73.8 ( <i>n</i> =132)	73.9–100 ( <i>n</i> =177)
Population density (people per square kilometer)	0–31.6 ( <i>n</i> =50)	31.7–146.5 ( <i>n</i> =48)	146.6–461.9 ( <i>n</i> =97)	462–31,431 ( <i>n</i> =253)

than 13 and 21 percent occurrence of any of the 84 commonly occurring compounds in samples from watersheds in the third and fourth quartiles of urban and agricultural land use (fig. 17A), respectively. These quartiles represent the national population of rivers with 17.1 percent or more urban and agricultural land use (quartiles 3 and 4; table 7) within their watersheds. Rivers with 3.2 to 17 percent urban and agricultural land use (quartile 2; table 7) had a median detection frequency of about 6 percent.

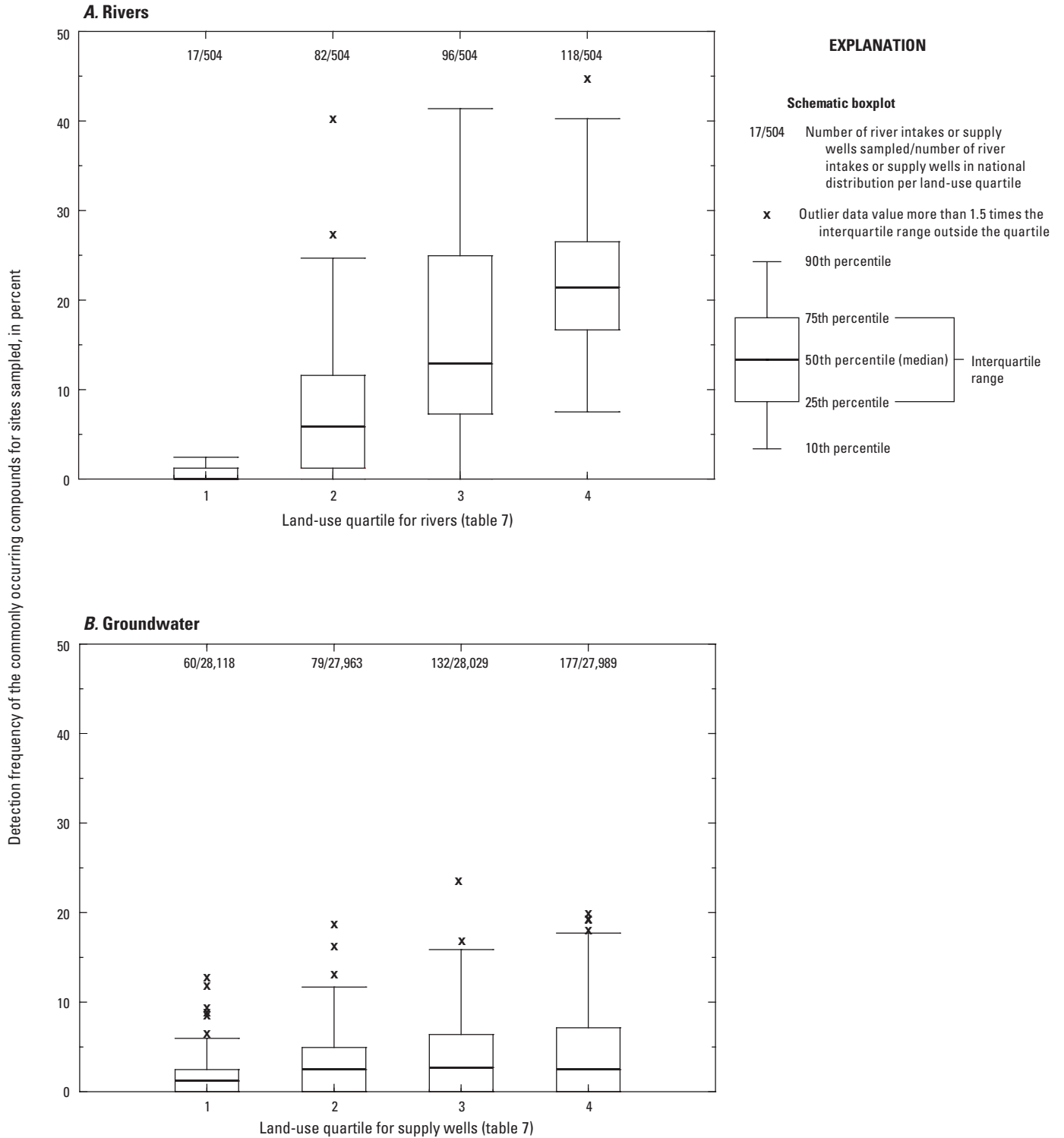
For groundwater, the median detection frequency for the commonly occurring compounds was lowest for the quartile with the least amount of urban and agricultural land and increased slightly from the second to third quartiles (fig. 17B). The difference in occurrence between the second, third, and fourth quartiles was small with median detection frequencies of about 3 percent in each of those quartiles. Urban and agricultural land use within the 500-m buffers around wells in these quartiles ranged from 18.7 to 100 (table 7).

Previous national assessments have shown that herbicide and herbicide degradates occur more frequently in rivers within an agricultural land-use setting (Gilliom and others, 2006). Similarly, solvents have been shown to occur more frequently in groundwater within an urban land-use setting than in any other land-use type (Zogorski and others, 2006). These studies focused primarily on ambient streams and shallow groundwater and were not specifically characterizing the quality of source water. However, findings herein compare favorably to previous assessments. This may indicate findings

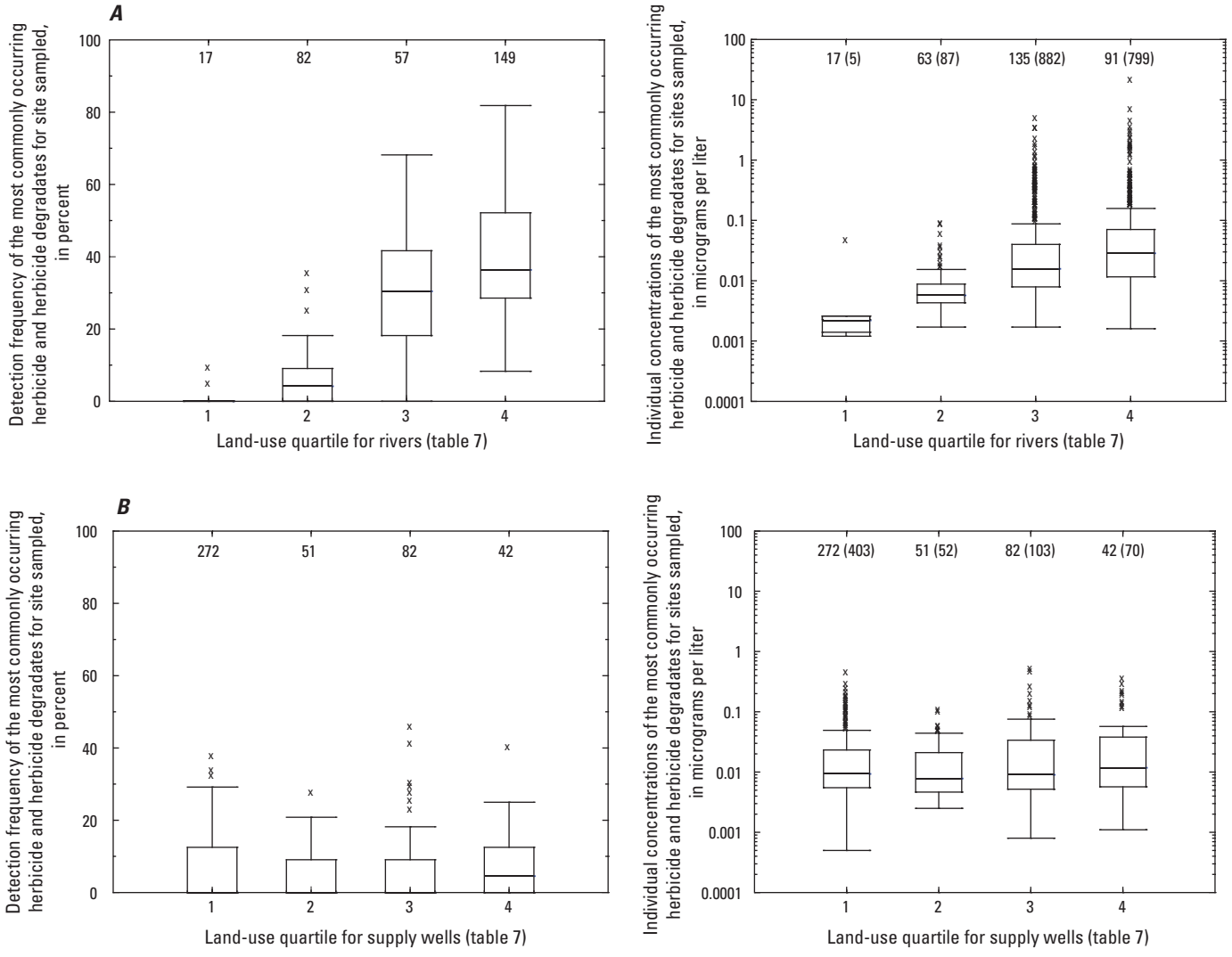
from ambient resource assessments are applicable to source waters used by community water systems (CWSs).

The increase in detection frequency of herbicides and herbicide degradates with increasing agricultural land use was more evident for rivers than for supply wells (fig. 18). For rivers, the median detection frequency increased for each quartile, with more than 30 and 36 percent occurrence of any of the 24 commonly occurring herbicides in samples from watersheds in the third and fourth quartiles of agricultural land use, respectively; collectively representing rivers with 9.1 percent or more agricultural land use within their watersheds (table 7; fig. 18A). The increase in each quartile indicates a strong correlation between the occurrence of herbicides and the amount of agricultural land use within the watershed. Similar to detection frequency, the median concentrations of herbicides and herbicide degradates in rivers increased as the amount of agricultural land use increased (fig. 18A). However, concentrations were low with median concentrations in the fourth quartile (most agricultural land) of about 0.03 µg/L.

The occurrence of herbicides and herbicide degradates generally did not change with increasing agricultural land use within the contributing area for the supply well (fig. 18B). The median detection frequency was much less than 1 percent in the first three quartiles compared to about 5 percent in the fourth quartile. This slight increase in the fourth quartile indicates that wells located in areas with the largest amount of agricultural land use may be more susceptible to herbicides. When detected, the concentrations of herbicides and herbicide degradates in all four quartiles were low with a median



**Figure 17.** Detection frequency without an assessment level of commonly detected compounds within urban and agricultural land-use quartiles for 2,016 river intakes and 112,099 supply wells considered to represent the national distribution of river intakes and supply wells, respectively, supplying community water systems for *A*, rivers and *B*, supply wells.



**EXPLANATION**

**Schematic boxplot**

- 17 Number of samples from river intakes or supply wells
  - 17 (5) Number of samples from river intakes or supply wells (number of detections)
  - x Outlier data value more than 1.5 times the interquartile range outside the quartile
  - 90th percentile
  - 75th percentile
  - 50th percentile (median)
  - 25th percentile
  - 10th percentile
- Interquartile range

**Figure 18.** Occurrence and concentrations without an assessment level for commonly occurring herbicide and herbicide degradates within agricultural land-use quartiles for 2,016 river intakes and 112,099 supply wells considered to represent the national distribution of river intakes and supply wells, respectively, supplying community water systems for *A*, rivers and *B*, supply wells.

concentration of about 0.01  $\mu\text{g/L}$  (fig. 18B). These results indicate that concentrations of herbicides and herbicide degradates vary minimally in groundwater regardless of the percentage of agricultural land use in the contributing area. Compound detections can decrease with well depth (Hopple and others, 2009), but this relation was not evaluated for this report.

The occurrence of solvents did not change substantially with increasing urban land use for rivers or supply wells (fig. 19). For rivers, the median detection frequency increased only in the fourth quartile, with more than 8 percent occurrence of any of the 13 commonly occurring solvents in surface-water samples in the fourth quartile of urban land use (fig. 19A). When detected, the concentrations in all four quartiles were low with a median concentration of about 0.02  $\mu\text{g/L}$  (fig. 19A). These results indicate that concentrations of solvents remain the same in surface water regardless of the percentage of urban land use in the watershed.

Although the range of occurrence and concentrations of solvents increased from one quartile to the next for rivers and supply wells, changes were slightly more evident for supply wells (fig. 19B). The increasing range in each quartile indicates that wells located in areas with the largest amount of urban land use may be susceptible to solvents. The median solvent concentration in the fourth quartile for supply wells (0.08  $\mu\text{g/L}$ ) was slightly higher than for river intakes (fig. 19B). These results indicate that as the percentage of urban land use increases in the contributing area, the concentration ranges for solvents increase.

Commonly occurring herbicides and herbicide degradates and commonly occurring solvents were separately put into context with the national distribution of river intakes and supply wells used by CWSs. Each of the sites was grouped into the respective national population of urban and agricultural land-use quartiles, and trends in occurrence and concentrations were assessed. In general, the increase in detection frequency of the most commonly occurring compounds associated with increasing amounts of agricultural and urban land use for both rivers and supply wells highlights the importance of source water and wellhead protection strategies.

## Mixtures in Surface Water and Groundwater

In addition to assessing the occurrence of individual compounds in source-water samples from surface water and groundwater, the occurrence and characteristics of mixtures in these samples also were evaluated. Human exposure to compounds is rarely limited to a single compound, and so more emphasis recently has been placed on health risks from exposure to mixtures (Hasegawa and others, 1994; Yang, 1994; Toccalino and others, 2010; Toccalino and others, 2012).

As a first step toward evaluating the potential importance of mixtures of AOCs to source-water quality, a basic co-occurrence analysis was completed using no assessment level. Although nearly all single-sample concentrations of individual compounds detected were low (median detected concentration less than 0.03  $\mu\text{g/L}$ ), most samples contained mixtures of two

or more compounds (fig. 20). In surface water, approximately 86 percent of source-water samples contained two or more compounds, and 50 percent of samples contained at least 14 compounds. Twenty-five percent of samples contained at least 22 compounds. In groundwater, 50 percent of samples contained at least three compounds. Twenty-five percent of samples contained at least six compounds.

The co-occurrence analyses also were completed for surface water and groundwater using an assessment level of 0.05  $\mu\text{g/L}$  (fig. 20). At least 4 compounds in surface water and at least 1 compound in groundwater were detected in 50 percent of samples with an assessment level. The additional compounds found to co-occur as mixtures when not using an assessment level for both surface water and groundwater highlights the significance of low-level compound co-occurrence.

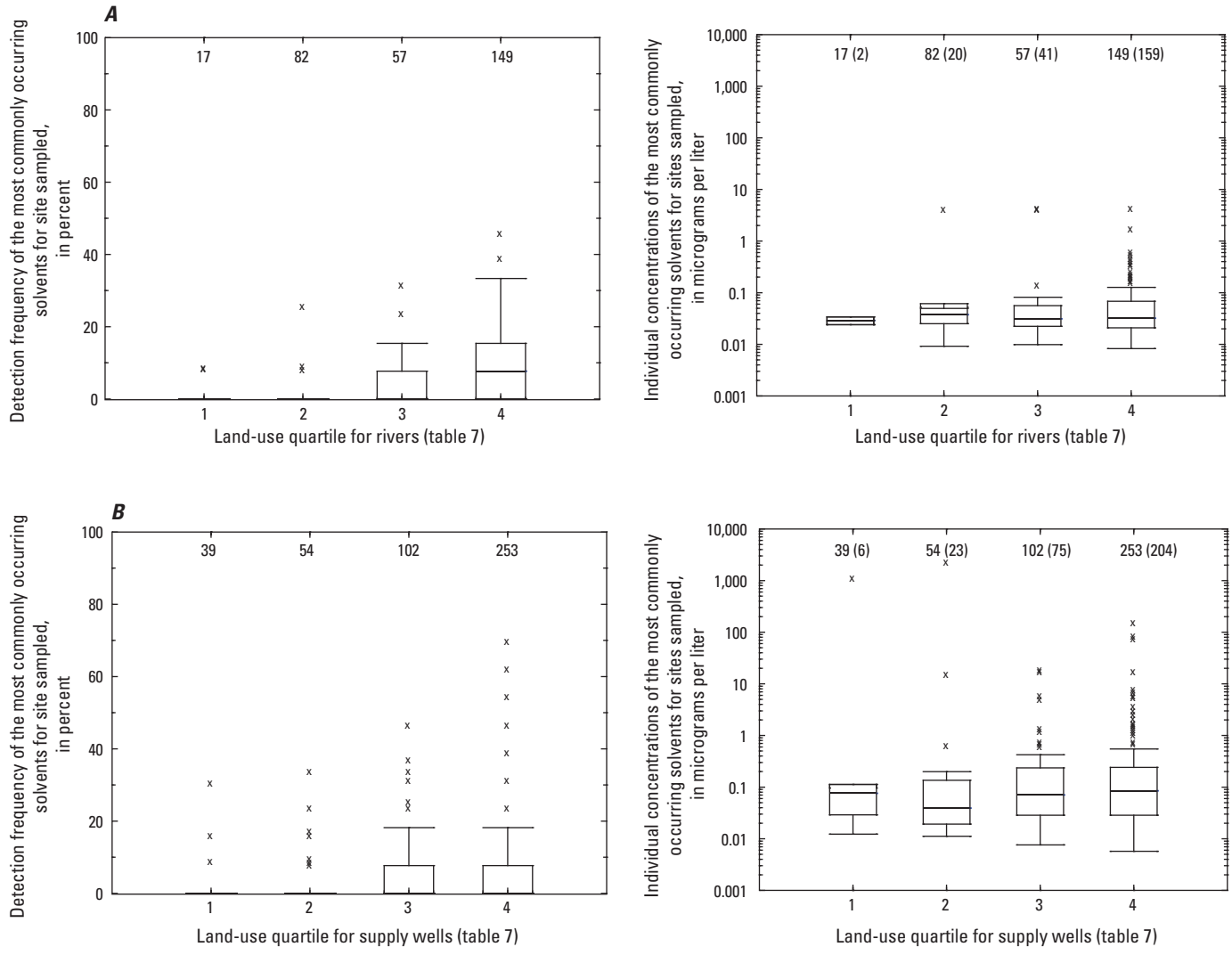
With respect to unique mixtures, the most commonly occurring compounds were examined in two categories: with and without an assessment level. Characterizing mixtures in these categories will begin to explain the most important compounds monitored that typically co-occur as a mixture in surface water and groundwater.

Using an assessment level of 0.05  $\mu\text{g/L}$  for the 25 most commonly occurring compounds, the 10 most frequently co-occurring mixtures in surface water include combinations of herbicides and herbicide degradates and the personal-care product HHCB (fig. 21). The combination of atrazine and 2-hydroxyatrazine (detected in 18 percent of samples) was the most frequent, followed by atrazine and deethylatrazine (17 percent), and HHCB and chloroform (16 percent). Atrazine occurred at concentrations within one-tenth of a benchmark (appendix 4).

The 10 most frequently co-occurring mixtures in groundwater (fig. 21) include combinations of solvents, disinfection by-products, and the gasoline oxygenate MTBE. The combination of chloroform and PCE (detected in 6.4 percent of samples) was the most frequent, followed by PCE and TCE (4.6 percent) and chloroform and MTBE (4.2 percent). Chloroform, PCE, and TCE also occurred at concentrations within one-tenth of a benchmark (appendix 5). In general, the compounds detected most frequently as individual compounds in the environment often composed the most frequent unique mixtures.

Characterizing the mixtures with an assessment level attempts to alleviate any potential bias because of varying LRLs between different compounds and identifies the most frequently occurring unique mixtures of compounds at concentrations equal to or greater than 0.05  $\mu\text{g/L}$ . In general, detection frequency depends on the LRL for each compound monitored. Thus, different detection frequencies for compounds with different LRLs may not represent true differences in water quality, but rather they may only reflect differences in analytical sensitivity among the different compounds.

Using no assessment level for the 25 most frequently occurring compounds, the 10 most frequently co-occurring mixtures in surface water include combinations of herbicides and herbicide degradates and chloroform. The combination

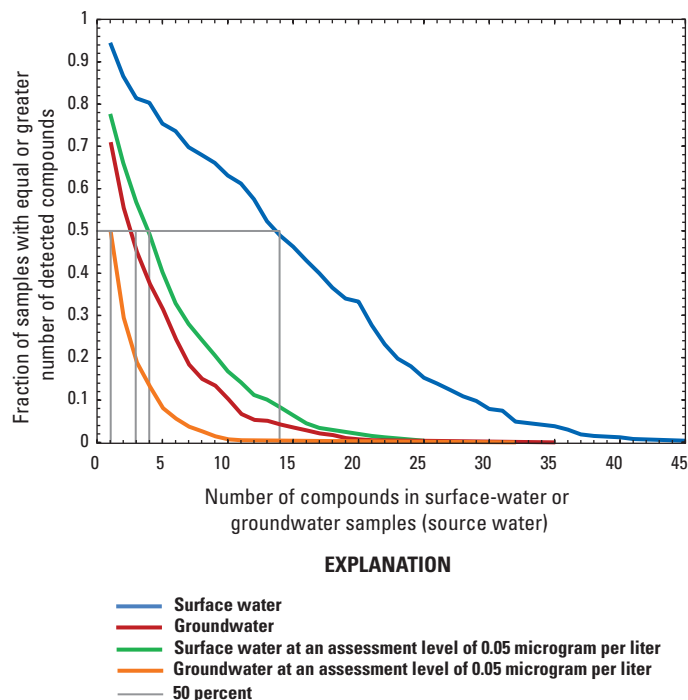


**EXPLANATION**

**Schematic boxplot**

- 17 Number of samples from river intakes or supply wells
  - 39 (6) Number of samples from river intakes or supply wells (number of detections)
  - x Outlier data value more than 1.5 times the interquartile range outside the quartile
- 90th percentile
- 75th percentile
- 50th percentile (median)
- 25th percentile
- 10th percentile
- Interquartile range

**Figure 19.** Occurrence and concentrations without assessment level of commonly occurring solvents within urban land-use quartiles for 2,016 river intakes and 112,099 supply wells considered to represent the national distribution of river intakes and supply wells, respectively, supplying community water systems for *A*, rivers and *B*, supply wells.



**Figure 20.** Distribution of the number of co-occurring anthropogenic organic compounds in surface water or groundwater samples collected during 2002–10 with and without a common assessment level.

of atrazine and deethylatrazine (59 percent) was the most frequent, followed by atrazine and simazine (57 percent) and atrazine and chloroform (53 percent) (fig. 22). Atrazine, simazine, and chloroform occurred at concentrations within one-tenth of a benchmark (appendix 4). The 10 most frequently co-occurring mixtures in groundwater include combinations of herbicides and herbicide degradates, chloroform, and PCE. The combination of atrazine and deethylatrazine (26 percent) was the most frequent, followed by chloroform and deethylatrazine (about 20 percent) and atrazine and chloroform (about 17 percent) (fig. 22). Atrazine, chloroform, and PCE occurred at concentrations within one-tenth of a benchmark (appendix 5). Determining the commonly occurring compounds that were part of a unique mixture without an assessment level will characterize compounds that are found to frequently co-occur at low concentrations (micrograms per liter or parts per billion) in the environment. Some compounds, such as simazine, were frequently detected at low concentrations in both surface water and groundwater (median concentrations 0.02  $\mu\text{g/L}$  and 0.006  $\mu\text{g/L}$ , respectively). In general, the compounds detected most frequently as individual compounds in the environment often composed the most frequent unique mixtures.

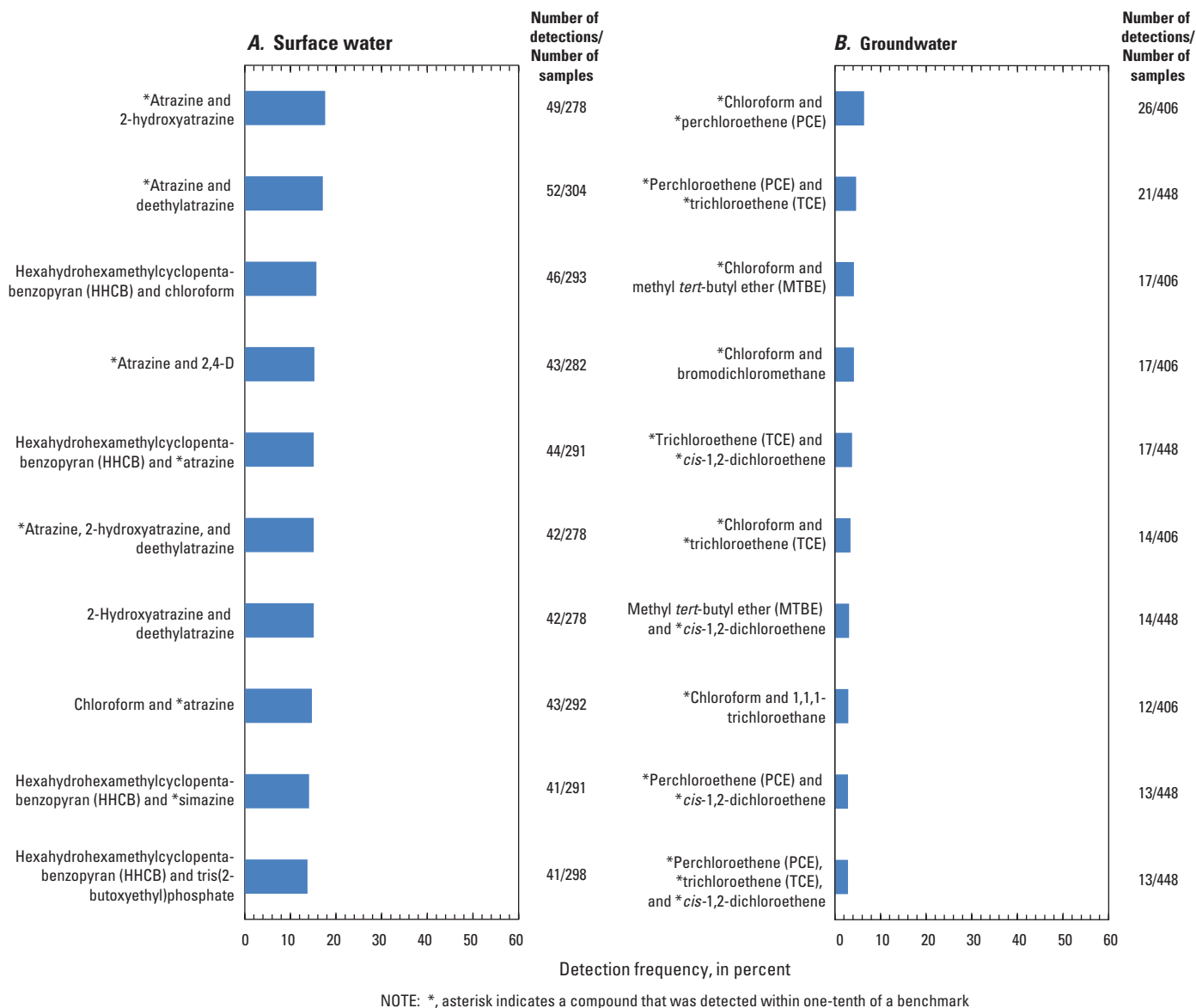
When evaluating unique mixtures of compounds without an assessment level, herbicide and herbicide degradates were among the most common compounds in the unique mixtures along with the disinfection by-product chloroform. This analysis begins to capture the significance of monitoring for degradates and, more specifically, for deethylatrazine, which is the

degradate compound of atrazine. For both surface water and groundwater, the results indicate that the most common unique compounds in each category were atrazine and chloroform. The presence of atrazine could be attributed to its widespread use as an agricultural pesticide (Kingsbury and others, 2008), and the presence of chloroform could be attributed to leakage of chlorinated water from distribution systems used for drinking water or wastewater sewers, swimming pools, and spas; chlorinated water used to irrigate lawns, golf courses, parks, gardens, and other areas; septic systems; and regulated discharge of chlorinated waters to recharge facilities (Ivahnenko and Barbash, 2004; Carter and others, 2012). Lastly, 5 of the 10 most frequently co-occurring unique mixtures were the same in surface-water and groundwater samples (fig. 22). The similar mixtures include (1) atrazine and deethylatrazine, (2) atrazine and simazine, (3) atrazine and chloroform, (4) simazine and deethylatrazine, and (5) atrazine, simazine, and deethylatrazine. No mixtures were similar between surface water and groundwater when an assessment level was used in evaluating these co-occurring compounds (fig. 21). Because similar mixtures were identified in both surface water and groundwater without using an assessment level, future studies could be directed toward better understanding the toxicological importance of these unique mixtures.

## Occurrence of Herbicides and Herbicide Degradates

In addition to the 265 compounds monitored at all sites, an additional 19 herbicides and herbicide degradates (3 herbicides and 16 degradates) were monitored at a subset of sites because the parent herbicide was likely to have been used in the study area and because of the higher potential for these degradates to persist at similar or greater concentrations relative to the parent compound (Thurman and others, 1992; Kalkhoff and others, 1998). The additional 19 herbicides and herbicide degradates (appendix 1) were analyzed in samples from 8 river intakes and at 118 supply wells. The 3 additional parent herbicides are dimethenamid, flufenacet, and propachlor. Degradates include dimethenamid ethane sulfonic acid (ESA), dimethenamid oxanilic acid, flufenacet ESA, flufenacet oxanilic acid, propachlor ESA, and propachlor oxanilic acid. Some of the additional herbicide degradates are degradates of three parent herbicides included as part of the 265 compounds monitored at all sites. These include (1) alachlor ESA 2nd amide, alachlor ESA, alachlor oxanilic acid, and alachlor sulfynilacetic acid (degradates of alachlor); (2) acetochlor oxanilic acid, acetochlor sulfynilacetic acid, acetachlor ESA, acetochlor/metolachlor ESA 2nd amide (degradates of acetachlor); and (3) metolachlor ESA and metolachlor oxanilic acid (degradates of metolachlor).

Two additional degradates of alachlor (2,6-diethylaniline and 2-chloro-2,6-diethylacetanilide) were analyzed as part of the 265 compounds monitored at all sites. Similarly, atrazine and four of its degradates (2-hydroxyatrazine, deethylatrazine,



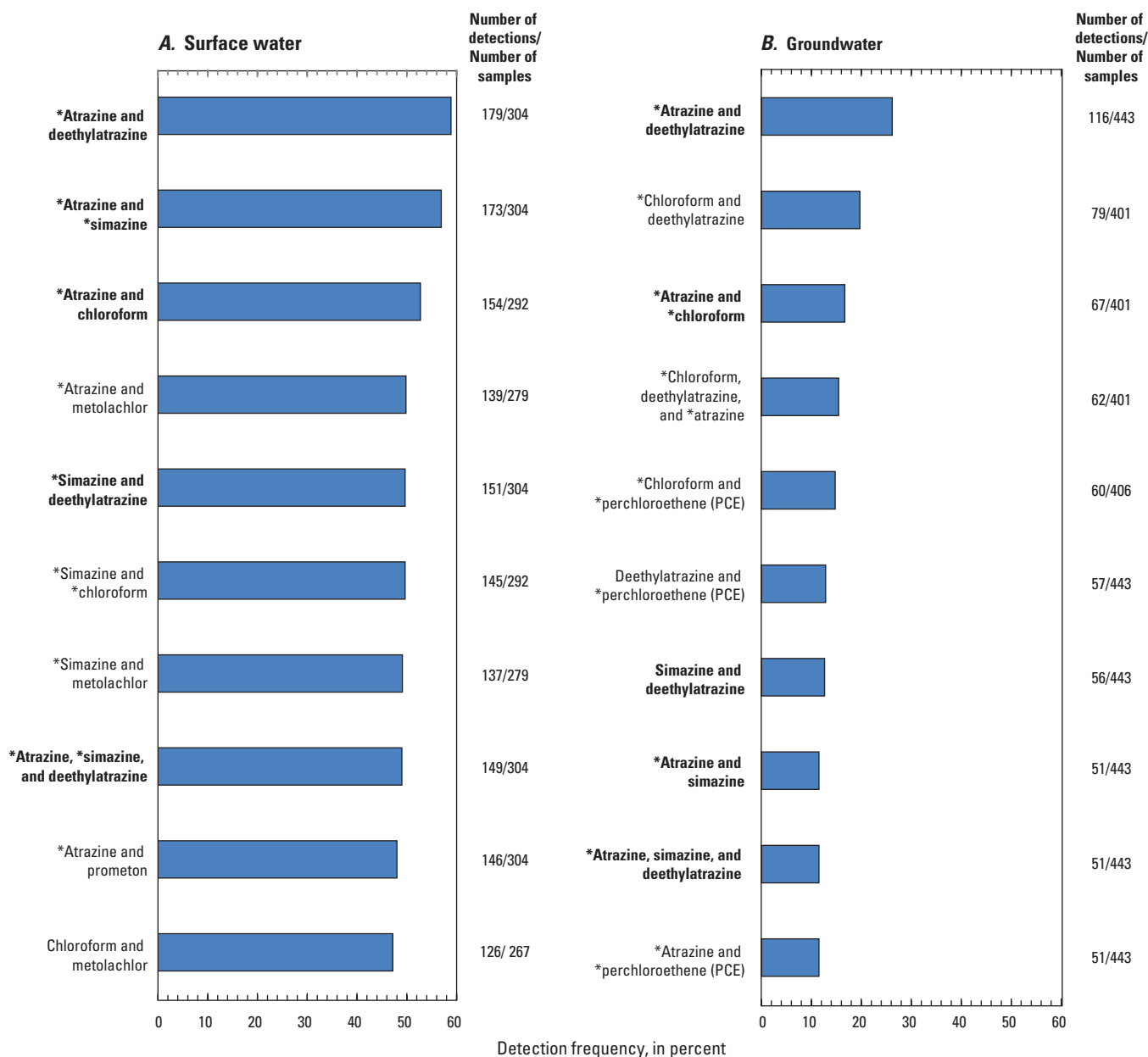
**Figure 21.** Ten most frequently co-occurring compounds evaluated with an assessment level of 0.05 microgram per liter in samples collected from *A*, surface water during 2002–10 and *B*, groundwater during 2002–09.

deethyldeisopropylatrazine, and deisopropylatrazine) were analyzed in samples collected at all sites. In total, data from 7 parent herbicides and 22 herbicide degradates were available for evaluation at 8 river intakes and 118 supply wells. These 7 parent herbicides are classified as anilides (flufenacet), amides (dimethenamid), chloroacetanilides (alachlor, acetochlor, metolachlor, and propachlor), and triazine (atrazine).

The summed concentrations of the degradates compared to concentrations of the seven respective parent herbicides in surface water and groundwater are shown in figure 23. The summed concentrations of the four atrazine degradates were similar to or slightly less than atrazine concentrations in surface water and were similar to or greater than atrazine concentrations in groundwater (fig. 23).

The summed concentrations of chloroacetanilide herbicide degradates in both surface water and groundwater were greater than the parent herbicide concentrations (fig. 23). In surface water, both the parent and degradates of chloroacetanilides commonly were present in samples; however, degradates of alachlor and acetochlor were occasionally present without their parent. This differs from groundwater, wherein degradates of metolachlor and alachlor were almost solely present without their parent. This may be due to the parent compound being present in groundwater for a longer period of time allowing it to more completely degrade. Acetochlor sulfynilacetic acid and alachlor sulfynilacetic acid were not detected in groundwater samples but were detected in surface-water samples. Propachlor and





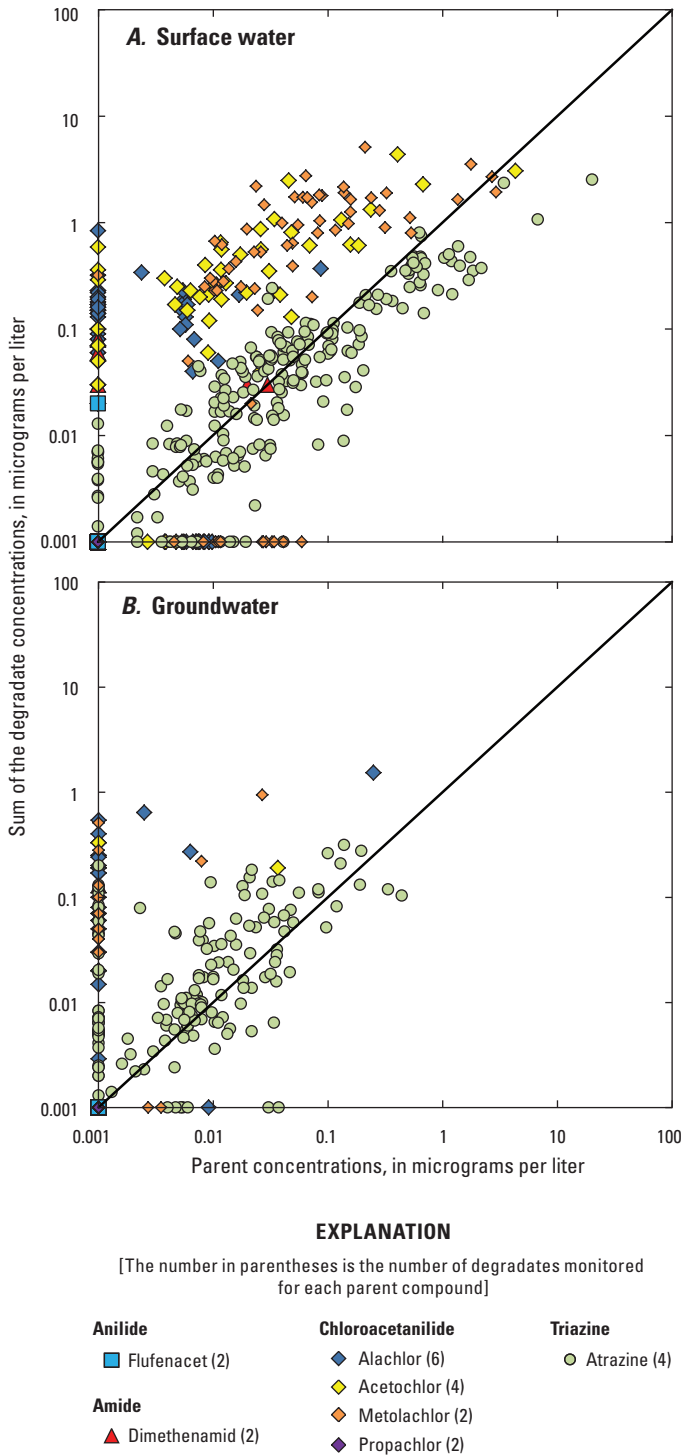
NOTE: Bold font indicates similar mixtures for surface water and groundwater at no assessment level; \*, asterisk indicates a compound that was detected within one-tenth of a benchmark

**Figure 22.** Ten most frequently co-occurring compounds evaluated without an assessment level in samples collected from *A*, surface water during 2002–10 and *B*, groundwater samples during 2002–09.

its degradates were the only chloroacetanilides that were not detected in either surface-water or groundwater samples.

Dimethenamid and flufenacet, along with their degradates, were infrequently detected (in about 1 percent of samples) in surface water or groundwater. Degradates of dimethenamid and the parent occurred at two surface-water sites and were never detected in groundwater. The degradates of flufenacet occurred in surface-water samples without the parent.

Understanding the persistence and degradation of parent compounds is important because herbicide degradates have been reported to have, at times, similar or greater concentrations compared to the parent compound in a sample (Hopple and others, 2009). The toxicity to humans for many of these degradate products is largely unknown and thus points to the importance of monitoring these compounds (both the parents and degradates) in the environment (Toccalino and Hopple, 2010). In addition, the co-occurrence of parent herbicides,



**Figure 23.** Relation between summed concentrations of herbicide degradates and concentrations of the parent herbicide for *A*, surface water, and *B*, groundwater.

primarily atrazine, metolachlor, acetochlor, and alachlor along with their respective degradates is important to monitor as these were detected in source waters of CWSs supplied by surface water. Similarly, degradates of metolachlor, alachlor, and atrazine are especially important to monitor for CWSs supplied by groundwater as they often occur without their parent.

## Summary and Conclusions

Drinking water delivered by community water systems (CWSs) comes from one or both of two sources: surface water and groundwater. Source water is raw, untreated water used by CWSs and is usually treated before distribution to consumers. Characterizing sources of drinking water is important to better understand what compounds may enter the treatment process either through natural occurrence in the environment, animal activity, or as a result of anthropogenic effects. Beginning in 2002, the U.S. Geological Survey’s (USGS) National Water-Quality Assessment Program initiated Source Water-Quality Assessments at select CWSs across the United States. The primary emphasis of Source Water-Quality Assessments is to characterize the occurrence of a large number of anthropogenic organic compounds that are predominantly unregulated by the U.S. Environmental Protection Agency in sources of drinking water.

As part of this effort, source-water samples from CWSs were collected during 2002–10 from 20 surface-water sites (river intakes) and during 2002–09 from 448 groundwater sites (supply wells). Rivers were sampled approximately 16 times over the course of a year, and supply wells were sampled once. Samples collected from all surface-water and groundwater sites were analyzed for 265 anthropogenic organic compounds. An additional 3 herbicides and 16 herbicide degradates were analyzed in samples collected from sites in areas where these compounds likely had been used. Of the 265 compounds monitored, 37 compounds have an established U.S. Environmental Protection Agency (EPA) Maximum Contaminant Level (MCL) for drinking water, 123 have USGS Health-Based Screening Levels (HBSLs), and 29 are included on the EPA Contaminant Candidate List 3 (CCL3). All compounds detected in source water were evaluated both with and without an assessment level and were grouped into 13 categories (hereafter termed as “use groups”) based on their primary use or source.

The CWS sites were characterized in a national context using an extract of the EPA Safe Drinking Water Information System to develop spatially derived and system-specific ancillary data. CWS information is contained in the Public Supply Database, which includes 2,016 active river intakes and 112,099 active supply wells. Ancillary variables including population served, watershed size, land use, population density, and recharge were characterized for each of the watersheds for river intakes and contributing areas for supply wells.

A total of 313 surface-water samples were collected from 20 river intakes. Seventy-one compounds from 12 of the 13 use groups were found to commonly occur (detected in greater than or equal to 1 percent of samples using an assessment level of 0.05 microgram per liter ( $\mu\text{g/L}$ ) or when a compound was detected in greater than or equal to 10 percent of samples without an assessment level) indicating a wide variety of sources and pathways to these rivers and highlighting the importance of source-water protection strategies. Using a common assessment level of 0.05  $\mu\text{g/L}$ , 15 of the 265 AOCs were detected in more than 10 percent of surface-water samples. Hexahydrohexamethylcyclopentabenzopyran (HHCB) was the most commonly occurring compound (29.5 percent) followed by chloroform (27.3 percent), atrazine (27.3 percent), tri(2-butoxyethyl)phosphate (23.8 percent), methyl *tert*-butyl ether (MTBE) (20.9 percent), and 2,4-D (20.4 percent). Most concentrations without an assessment level (63 percent) were less than 0.05  $\mu\text{g/L}$ .

A total of 448 groundwater samples were collected from supply wells that were sampled once during 2002–09 as part of 30 independent groundwater studies. Each independent groundwater study sampled about 15 CWS wells. Twenty-eight compounds from 7 of the 13 use groups commonly occurred indicating that a wide variety of sources and pathways exist for these compounds to reach these wells and highlighting the importance of wellhead protection strategies. Using the common assessment level of 0.05  $\mu\text{g/L}$ , 3 of the 265 AOCs were detected in more than 10 percent of groundwater samples. Chloroform was the most commonly occurring compound (23.9 percent) followed by MTBE (12.3 percent) and perchloroethene (11.6 percent). These compounds are among the most frequently occurring compounds found in national ambient resources assessment conducted by the USGS. This may indicate that compounds found to frequently occur in broad-scale resource assessments also may be present in source water. Most concentrations without an assessment level (61 percent) were less than 0.05  $\mu\text{g/L}$ .

About one-half the 265 compounds monitored (122) were detected in both surface-water and groundwater samples without using an assessment level. This highlights the importance of monitoring source water supplied by both water types to identify compounds that may occur most frequently, especially those compounds that are unregulated. About 28 percent (73 of 265) of the compounds were never detected in either type of water samples. Fourteen percent (36) of compounds were detected only in surface-water samples, whereas 13 percent (34) were detected only in groundwater samples. Many compounds that were detected frequently were found to occur in both water types, further indicating that these compounds have a variety of sources and pathways to enter water supplies.

A more diverse suite of compounds was detected in surface water than groundwater. However, the herbicides and herbicide degradate group was the most frequent group of compounds detected in both surface water and groundwater. Sixty-five of the most commonly occurring compounds were detected in one or more samples from both surface water and

groundwater. For commonly occurring compounds detected in both water types, the detection frequency was higher for surface-water samples than groundwater samples; however, concentrations were not significantly different (rank-sum test;  $p$ -value=0.4292). Different patterns in concentrations were observed for analyses of individual use groups. For example, herbicides and herbicide degradates and personal-care products were detected more frequently and concentrations were greater in surface-water samples than in groundwater samples. Some solvents and disinfection by-products were detected more frequently in surface water, whereas others were detected more frequently in groundwater, and yet concentrations for both use groups were larger in groundwater. This highlights the importance of understanding the sources and pathways for a compound to enter source water as well as the compound's physical and chemical properties.

Four compounds (acetochlor, diuron, MTBE, and metolachlor) in surface water and three compounds (1,1-dichloroethane, diuron, and MTBE) in groundwater that commonly occurred are included on the CCL3. The gasoline oxygenate MTBE was detected more frequently in surface water (24 percent) than in groundwater (15 percent). Similarly, the herbicide diuron was detected more frequently in surface water (35 percent) than in groundwater (9 percent). The frequent occurrence without an assessment level of these two compounds in surface-water and groundwater samples may warrant consideration in future monitoring programs.

Human-health benchmarks (MCLs for regulated compounds and HBSLs for unregulated compounds) were available for more than one-half the compounds (160 of the 265) analyzed in this study. Fifty-eight percent (41 of 71) of the commonly occurring compounds in surface water have a human-health benchmark to which concentrations can be compared: 19 have MCLs and 22 have HBSLs. Five compounds (4 herbicides and herbicide degradates and 1 insecticide) in surface water had concentrations that were greater than or within one-tenth of a benchmark. No commonly occurring compounds had an annual mean concentration greater than or within one-tenth of the benchmark value. Eighty-three percent (24 of 28) of the most commonly occurring compounds in groundwater have a human-health benchmark for which concentrations can be compared: 14 have MCLs and 10 have HBSLs. Nine compounds (1 disinfection by-product, 1 herbicide, 1 organic synthesis compound, and 6 solvents) had concentrations in groundwater that were greater than or within one-tenth of a benchmark. Perchloroethene and trichloroethene were the only compounds with concentrations in groundwater greater than the benchmark value. Although more compounds were detected in surface water and occurred more frequently than in groundwater, the number of compounds detected within at least one-tenth of a benchmark was roughly double in groundwater (9) than rivers (5).

Thirty-two of the commonly occurring compounds in surface water and groundwater do not have a human-health benchmark. Of these, 17 were detected in 10 percent or more source-water samples from either water type. Two compounds

were found to occur in more than 10 percent of samples in both water types: deethylatrazine and MTBE. The frequent occurrence of these two compounds may warrant the development of appropriate toxicity information, which would allow the ability to calculate an HBSL value to which concentration data could be compared. Lacking this information, it is not possible to interpret results for these compounds in a human-health context.

To put results from this study into context with the national distribution of river intakes and supply wells used by CWSs, sites were grouped into the respective national population of land-use quartiles. The increase in compound occurrence with increasing urban and agricultural land use in the watershed or contributing area was more evident for rivers than for supply wells. For rivers, the median detection frequency of the most commonly detected compounds increased for each land-use quartile, with more than 13 and 21 percent compound occurrence in samples from watersheds in the third and fourth quartiles, respectively, of urban and agricultural land use combined. The third and fourth quartiles represent rivers with 17 percent or more urban and agricultural land use within their watershed. In groundwater, the difference in occurrence between the second, third, and fourth quartiles was small with median detection frequencies of about 3 percent in each.

The increase in detection frequency of herbicides and herbicide degradates with increasing agricultural land use was more evident for rivers than for supply wells. For rivers, the median detection frequency increased for each quartile, with more than 30 and 36 percent in samples from watersheds in the third and fourth quartiles of agricultural land use, respectively (collectively representing rivers with 9.1 percent or more agricultural land use within their watershed). Similarly, the median detected concentrations increased as the amount of agricultural land use increased; however, concentrations were low with median concentrations in the fourth quartile of about 0.03  $\mu\text{g/L}$ . The increased detection frequency from one quartile to the next indicates that there is a strong correlation between the occurrence of commonly occurring compounds, especially herbicides and herbicide degradates, and the percentage of urban and (or) agricultural land use within the watershed. The occurrence of solvents did not change substantially with increasing urban land use for rivers or supply wells.

Basic co-occurrence analyses were completed with and without an assessment level. Considering all detections in surface water without an assessment level, approximately 86 percent of source-water samples contained two or more compounds, and 50 percent of samples contained at least 14 compounds. Considering all detections in groundwater without an assessment level, 50 percent of samples contained at least three compounds. Using an assessment level of 0.05  $\mu\text{g/L}$ , 50 percent of samples contained at least 4 compounds in surface water and 1 compound in groundwater.

Characterizing the most frequently occurring unique mixtures was done with and without an assessment level. Summarizing mixtures with an assessment level attempts

to alleviate any potential bias because of varying laboratory reporting levels between different compounds and identifies the most frequently occurring unique mixtures of compounds at concentrations greater than or equal to 0.05  $\mu\text{g/L}$ . The 10 most frequently co-occurring mixtures, using an assessment level, in surface water include atrazine and 2-hydroxyatrazine (18 percent), atrazine and deethylatrazine (17 percent), and HCHB and chloroform (16 percent). The 10 most frequently co-occurring mixtures in groundwater include chloroform and perchloroethene (6.4 percent), perchloroethene and trichloroethene (4.6 percent), and chloroform and MTBE (4.2 percent). In general, the compounds detected most frequently as individual compounds in the environment often composed the most frequent unique mixtures.

Comparing the compounds that were part of a unique mixture without an assessment level characterizes compounds that frequently co-occur at low concentrations (micrograms per liter or parts per billion) in the environment. Using no assessment level, the 10 most frequently co-occurring mixtures in surface water include atrazine and deethylatrazine (59 percent), atrazine and simazine (57 percent), and atrazine and chloroform (53 percent). The 10 most frequently co-occurring mixtures in groundwater include atrazine and deethylatrazine (26 percent), chloroform and deethylatrazine (about 20 percent), and atrazine and chloroform (about 17 percent). This analyses captures the significance of monitoring pesticide degradates and, more specifically, deethylatrazine.

Five of the 10 most frequently co-occurring unique mixtures in both surface water and groundwater were the same: atrazine and deethylatrazine, atrazine and chloroform, simazine and deethylatrazine and simazine, atrazine and simazine, and atrazine, simazine, and deethylatrazine. No mixtures were similar between surface water and groundwater when an assessment level was used. Because similar mixtures were identified in both surface water and groundwater without using an assessment level, future studies could be directed toward better understanding the toxicological importance of these unique mixtures.

In addition to the 265 compounds monitored at all sites, an additional 19 herbicides and herbicide degradates (3 herbicides and 16 degradates) were monitored at a subset of sites because the parent herbicide was likely to have been used in the study area and because of the higher potential for these degradates to persist at similar or greater concentrations relative to the parent compound. The additional 19 herbicides and herbicide degradates were monitored at 8 river intakes and at 118 supply wells.

Concentrations of the summed concentrations of degradates were compared to the concentrations of parent herbicides in surface water and groundwater. In surface water, the summed concentrations of the four atrazine degradates (2-hydroxyatrazine, deethylatrazine, deethyldeisopropylatrazine, and deisopropylatrazine) were similar to or slightly less than the parent compound. In groundwater, the summed concentrations were similar to or greater than the parent compound. The summed concentrations of 14 chloroacetanilide

herbicide (alachlor, acetochlor, metolachlor, and propachlor) degradates in both surface water and groundwater was greater than the parent herbicide. In surface water, degradates of alachlor and acetochlor were occasionally present without their parent compounds. In groundwater, degradates of metolachlor and alachlor were almost solely present without their parent compounds. Acetochlor sulfynilacetic acid and alachlor sulfynilacetic acid were detected in surface water but not groundwater. Propachlor and the respective degradates were the only chloroacetanilides that were never detected in either surface water or groundwater. Dimethenamid and flufenacet, along with their degradates, were infrequently detected (about 1 percent) in surface water and groundwater.

The toxicity to humans for many of these degradate products is largely unknown and thus points to the importance of monitoring these compounds (both the parents and degradates) in the environment. In addition, the co-occurrence of parent herbicides, primarily atrazine, metolachlor, acetochlor, and alachlor, along with their degradates is important because these were detected in source waters of CWSs supplied by surface water. Similarly, degradates of metolachlor, alachlor, and atrazine are especially important for CWSs supplied by groundwater as they often occur without their parent.

This study highlights the importance of anthropogenic organic compounds in source water of select CWSs in the United States by characterizing the occurrence of the anthropogenic organic compounds in surface water and groundwater samples. Compound concentrations and occurrence are summarized and evaluated in a human-health context, when possible. Additionally, compounds found to co-occur as mixtures for both rivers and groundwater highlight the significance of low-level compound co-occurrence.

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**Appendix 1. Compounds Monitored, Chemical Abstract Service Registry Number (CASRN), Drinking-Water Benchmark, Primary Use or Source Group, and Analytical Schedule**

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Disinfection by-products (n=4)								
Bromodichloromethane	SH2020	75-27-4	32101	MCL <sup>b</sup>	NA	80	Trihalomethane, organic synthesis, fire extinguishers	Bender and others, 1999; U.S. National Library of Medicine, 2006.
Bromoform	SH2020	75-25-2	32104	MCL <sup>b</sup>	NA	80	Trihalomethane, solvent, pharmaceutical manufacturing, organic synthesis, fire extinguishers, heavy liquid for mineral separations, reagent for graphite ore extraction	Bender and others, 1999; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
Chloroform	SH2020	67-66-3	32106	MCL <sup>b</sup>	NA	80	Trihalomethane, fumigant, solvent, anaerobic degradate of carbon tetrachloride, used in synthesis of refrigerants, extractant, chemical intermediate	Egli and others, 1988; Bender and others, 1999; Scorecard, 2006; Zogorski and others, 2006.
Dibromochloromethane	SH2020	124-48-1	32105	MCL <sup>b</sup>	NA	80	Trihalomethane, organic synthesis, chemical intermediate for manufacture of aerosol propellants, refrigerant, pesticides, fire extinguishing agent	Bender and others, 1999; U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
Fumigant-related compounds (n=9)								
1,2-Dibromo-3-chloropropane (DBCP)	SH2020	96-12-8	82625	MCL	NA	0.2	Organic synthesis, nematocide	Budavari, 1989; Zogorski and others, 2006.
1,2-Dibromoethane (EDB)	SH2020	106-93-4	77651	MCL	NA	0.05	Anti-knock compound in gasoline, former pesticide, solvent, waterproofing preparations, dyes, and pharmaceuticals	Budavari, 1989; National Oceanic and Atmospheric Administration, 2008; Scorecard, 2006; U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
1,2-Dichloropropane	SH2020	78-87-5	34541	MCL	NA	5	Dry-cleaning solvent, chemical intermediate, stain remover	Budavari, 1989, 1996; Tesoriero and others, 2001; Zogorski and others, 2006.
1,3-Dichloropropane	SH2020	142-28-9	77173	NA	NA	--	Fumigant contaminant	Bender and others, 1999.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Tocalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Fumigant-related compounds (n=9)—Continued								
1,4-Dichlorobenzene (p-dichlorobenzene)	SH2020	106-46-7	34571	MCL	NA	75	Deodorizer, moth killer, manufacture of dyes, chemical intermediate	Bender and others, 1999; Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006.
2,2-Dichloropropane	SH2020	594-20-7	77170	NA	NA	--	Fumigant contaminant	Cohen and others, 1983; Bender and others, 1999.
Bromomethane (methyl bromide)	SH2020	74-83-9	34413	HBSL	CCL3	100	Solvent, chemical intermediate	Bender and others, 1999; Zogorski and others, 2006.
cis-1,3-Dichloropropene	SH2020	10061-01-5	34704	HBSL	NA	0.3-30	Solvent, chemical intermediate	Bender and others, 1999; Zogorski and others, 2006.
trans-1,3-Dichloropropene	SH2020	10061-02-6	34699	HBSL	NA	0.3-30	Solvent, chemical intermediate	Bender and others, 1999; Zogorski and others, 2006.
Fungicides and fungicide degradates (n=9)								
3,5-Dichloroaniline	SH2033	626-43-7	61627	NA	NA	--	--	Sandstrom and others, 2001.
Benomyl	SH2060	17804-35-2	50300	HBSL	NA	40	--	Furlong and others, 2001; Wood, 2010.
cis-Propiconazole	SH2033	c-60207-90-1 <sup>c</sup>	79846	HBSL	NA	70	--	Sandstrom and others, 2001.
Iprodione	SH2003/2033	36734-19-7	61593	HBSL	NA	0.8-80	--	Sandstrom and others, 2001; Wood, 2010.
Metalaxyl	SH2003/2033	57837-19-1	61596	HBSL	NA	500	--	Furlong and others, 2001; Glassmeyer and others, 2005; Wood, 2010.
Myclobutanil	SH2003/2033	88671-89-0	61599	HBSL	NA	200	--	Sandstrom and others, 2001; Wood, 2010.
Propiconazole	SH2060	60207-90-1	50471	HBSL	NA	70	--	Furlong and others, 2001; Wood, 2010.
Tebuconazole	SH2033	107534-96-3	62852	NA	CCL3	--	--	Wood, 2010.
trans-Propiconazole	SH2033	t-60207-90-1 <sup>c</sup>	79847	HBSL	NA	70	--	Sandstrom and others, 2001.
Gasoline hydrocarbons, oxygenates, and oxygenate degradates (n=27)								
1,2,3,4-Tetramethylbenzene	SH2020	488-23-3	49999	NA	NA	--	Petroleum hydrocarbon	Cozzarelli and others, 1994.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Gasoline hydrocarbons, oxygenates, and oxygenate degradates ( <i>n</i> =27)—Continued								
1,2,3,5-Tetramethylbenzene	SH2020	527–53–7	50000	NA	NA	--	Petroleum hydrocarbon	Cozzarelli and others, 1990.
1,2,3-Trimethylbenzene	SH2020	526–73–8	77221	NA	NA	--	Gasoline hydrocarbon, pesticide adjuvant	Wiedemeier and others, 1996; U.S. Environmental Protection Agency, 2009c.
1,2,4-Trimethylbenzene	SH2020	95–63–6	77222	NA	NA	--	Petroleum hydrocarbon, pesticide adjuvant, chemical intermediate	Cozzarelli and others, 1990; Wiedemeier and others, 1996; U.S. Environmental Protection Agency, 2009c; U.S. National Library of Medicine, 2006.
1,3,5-Trimethylbenzene	SH2020	108–67–8	77226	NA	NA	--	Used in synthesis of Ethanox 330, gasoline hydrocarbon	Wiedemeier and others, 1996; U.S. National Library of Medicine, 2006.
1-Ethyl-2-methylbenzene	SH2020	611–14–3	77220	NA	NA	--	Petroleum hydrocarbon	Cozzarelli and others, 1990; Zogorski and others, 2006.
1-Methylnaphthalene	SH1433	90–12–0	62054	NA	NA	--	Polynuclear aromatic hydrocarbon, pesticide adjuvant, wall coverings, gasoline and diesel fuel component	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
2,6-Dimethylnaphthalene	SH1433	581–42–0	62055	NA	NA	--	Polynuclear aromatic hydrocarbon, diesel fuel component, pesticide adjuvant, insecticide	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
2-Methylnaphthalene	SH1433	91–57–6	62056	HBSL	NA	30	Polynuclear aromatic hydrocarbon, pesticide adjuvant, sealants, adhesives, wall coverings, gasoline and diesel fuel component	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
Benzene	SH2020	71–43–2	34030	MCL	NA	5	Gasoline hydrocarbon, organic synthesis	Bender and others, 1999; U.S. National Library of Medicine, 2006.
Diisopropyl ether (DIPE)	SH2020	108–20–3	81577	NA	NA	--	Gasoline oxygenate, solvent	Bender and others, 1999.



**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Gasoline hydrocarbons, oxygenates, and oxygenate degradates (n=27)—Continued								
Ethyl <i>tert</i> -butyl ether (ETBE)	SH2020	637-92-3	50004	NA	NA	--	Gasoline oxygenate	Bender and others, 1999.
Ethylbenzene	SH2020	100-41-4	34371	MCL	NA	700	Gasoline hydrocarbon, organic synthesis, solvent, pesticide adjuvant	Bender and others, 1999; U.S. National Library of Medicine, 2006; U.S. Environmental Protection Agency, 2009c.
Isopropylbenzene	SH2020	98-82-8	77223	HBSL	NA	700	Organic synthesis, building materials, solvent, gasoline hydrocarbon, intermediate in production of plastics	Bender and others, 1999; Glassmeyer and others, 2005.
<i>m</i> - & <i>p</i> -Xylene	SH2020	<i>m</i> : 106-42-3; <i>p</i> : 108-38-3	85795	MCL <sup>d</sup>	NA	10,000	Gasoline hydrocarbon, solvent, organic synthesis	U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
Methyl <i>tert</i> -butyl ether (MTBE)	SH2020	1634-04-4	78032	NA	CCL3	--	Gasoline oxygenate	Bender and others, 1999.
Naphthalene	SH2020	91-20-3	34696	HBSL	NA	100	Polynuclear aromatic hydrocarbon, petroleum hydrocarbon, pesticide adjuvant, combustion product, disinfectant, antiseptic, mouthwash, throat lozenges, slimicides, manufacture of synthetic fibers, fumigant, moth repellent	Bender and others, 1999; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
<i>n</i> -Butylbenzene	SH2020	104-51-8	77342	NA	NA	--	Solvent, organic synthesis	Bender and others, 1999; U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
<i>o</i> -Xylene	SH2020	95-47-6	77135	MCL <sup>d</sup>	NA	10,000	Gasoline hydrocarbon, pesticide adjuvant, organic synthesis, solvent	Bender and others, 1999; U.S. National Library of Medicine, 2006.
<i>p</i> -Isopropyltoluene ( <i>p</i> -cymene)	SH2020	99-87-6	77356	NA	NA	--	Organic synthesis, solvent, heat transfer agent, wood office furniture	Bender and others, 1999; Scorecard, 2006; U.S. National Library of Medicine, 2006.

**Appendix 1.** Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Gasoline hydrocarbons, oxygenates, and oxygenate degradates (n=27)—Continued								
<i>sec</i> -Butylbenzene	SH2020	135–98–8	77350	NA	CCL3	--	Gasoline hydrocarbon, solvent, organic synthesis, plasticizer	Bender and others, 1999; U.S. National Library of Medicine, 2006.
Styrene	SH2020	100–42–5	77128	MCL	NA	100	Organic synthesis, manufacture of styrofoam, building materials, adhesives	Bender and others, 1999; Scorecard, 2006; U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
<i>tert</i> -Amyl alcohol (2-methyl-2-butanol)	SH4024	75–85–4	77073	NA	NA	--	Gasoline oxygenate	U.S. Geological Survey, 2007b.
<i>tert</i> -Amyl methyl ether (TAME)	SH2020	994–05–8	50005	NA	NA	--	Gasoline oxygenate	Bender and others, 1999.
<i>tert</i> -Butyl alcohol	SH4024	75–65–0	77035	NA	NA	--	Gasoline oxygenate; methyl <i>tert</i> -butyl ether (MTBE) degradate	Pankow and others, 1996; Bradley and others, 2001; U.S. Geological Survey, 2007b.
<i>tert</i> -Butylbenzene	SH2020	98–06–6	77353	NA	NA	--	Organic synthesis	Bender and others, 1999; U.S. National Library of Medicine, 2006.
Toluene	SH2020	108–88–3	34010	MCL	NA	1,000	Solvent consumer products, pesticide adjuvant	Bender and others, 1999; U.S. Environmental Protection Agency, 2009c.
Herbicides and herbicide degradates (n=68)								
2,4-D	SH2060	94–75–7	39732	MCL	NA	70	--	Furlong and others, 2001.
2,4-D methyl ester	SH2060	1928–38–7	50470	NA	NA	--	--	Furlong and others, 2001.
2,4-DB	SH2060	94–82–6	38746	HBSL	NA	200	--	Furlong and others, 2001.
2,6-Diethylaniline	SH2003/2033	579–66–8	82660	NA	NA	--	Herbicide (mostly alachlor) degradate	Zaugg and others, 1995; Hladik and others, 2005.
2-Chloro-2,6-diethylacetanilide	SH2003/2033	6967–29–9	61618	NA	NA	--	Herbicide (mostly alachlor) degradate	Sandstrom and others, 2001; Hladik and others, 2005.
2-Ethyl-6-methyl-aniline	SH2003/2033	24549–06–2	61620	NA	NA	--	Herbicide (acetochlor or metolachlor) degradate	Sandstrom and others, 2001; Hladik and others, 2005.
2-Hydroxyatrazine	SH2060	2163–68–0	50355	HBSL	NA	70	Herbicide (atrazine) degradate	Furlong and others, 2001.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
3-(4-Chlorophenyl)-1-methyl urea	SH2060	5352-88-5	61692	NA	NA	--	Herbicide degradate	Furlong and others, 2001.
3,4-Dichloroaniline	SH2003/2033	95-76-1	61625	NA	NA	--	Herbicide (diuron) degradate	Sandstrom and others, 2001.
4-Chloro-2-methyl-phenol	SH2003/2033	1570-64-5	61633	NA	NA	--	Herbicide (MCPA) degradate	Sandstrom and others, 2001.
Acetochlor	SH2003/2033	34256-82-1	49260	HBSL	CCL3	10	--	Lee and Strahan, 2003.
Acifluorfen	SH2060	50594-66-6	49315	HBSL	NA	90	--	Furlong and others, 2001.
Alachlor	SH2003/2033	15972-60-8	46342	MCL	NA	2	--	Zaugg and others, 1995.
Atrazine	SH2003/2033	1912-24-9	39632	MCL	NA	3	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
Benfluralin	SH2003/2033	1861-40-1	82673	HBSL	NA	4	--	Zaugg and others, 1995.
Bensulfuron-methyl	SH2060	83055-99-6	61693	HBSL	NA	1,000	--	Furlong and others, 2001.
Bentazon	SH2060	25057-89-0	38711	HBSL	NA	200	--	Furlong and others, 2001.
Bromacil	SH2060	314-40-9	04029	HBSL	NA	70	--	Furlong and others, 2001; Glassmeyer and others, 2005.
Bromoxynil	SH2060	1689-84-5	49311	HBSL	NA	10	--	Furlong and others, 2001.
Chloramben, methyl ester	SH2060	7286-84-2	61188	NA	NA	--	--	Furlong and others, 2001.
Chlorimuron-ethyl	SH2060	90982-32-4	50306	HBSL	NA	600	--	Furlong and others, 2001.
Clopyralid	SH2060	1702-17-6	49305	HBSL	NA	1,000	--	Furlong and others, 2001.
Cyanazine	SH2033	21725-46-2	04041	HBSL	NA	1	--	Zaugg and others, 1995.
Cycloate	SH2060	1134-23-2	04031	HBSL	NA	40	--	Furlong and others, 2001.
Dacthal	SH2003/2033	1861-32-1	82682	HBSL	NA	70	--	Zaugg and others, 1995.
Dacthal monoacid	SH2060	887-54-7	49304	NA	NA	--	Herbicide (dacthal) degradate	Furlong and others, 2001.
Deethylatrazine	SH2003/2033	6190-65-4	04040	NA	NA	--	Herbicide (atrazine) degradate	Zaugg and others, 1995.
Deisopropylatrazine	SH2060	1007-28-9	04038	NA	NA	--	Herbicide (atrazine) degradate	Furlong and others, 2001.

**Appendix 1.** Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.—Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Herbicides and herbicide degradates (n=68)—Continued								
Dicamba	SH2060	1918-00-9	38442	HBSL	NA	3,000	--	Furlong and others, 2001.
Dichlorprop	SH2060	120-36-5	49302	HBSL	NA	300	--	Furlong and others, 2001.
Dinoseb	SH2060	88-85-7	49301	MCL	NA	7	Plant growth regulator	Furlong and others, 2001.
Diphenamid	SH2060	957-51-7	04033	HBSL	NA	200	--	Furlong and others, 2001.
Diuron	SH2060	330-54-1	49300	HBSL	CCL3	2-200	--	Furlong and others, 2001.
Eptam (EPTC)	SH2033	759-94-4	82668	HBSL	NA	200	--	Zaugg and others, 1995; Wood, 2010.
Fenuron	SH2060	101-42-8	49297	NA	NA	--	--	Furlong and others, 2001.
Flumetsulam	SH2060	98967-40-9	61694	HBSL	NA	7,000	--	Furlong and others, 2001.
Fluometuron	SH2060	2164-17-2	38811	HBSL	NA	4	--	Furlong and others, 2001.
Hexazinone	SH2003/2033	51235-04-2	04025	HBSL	NA	400	--	Sandstrom and others, 2001.
Imazaquin	SH2060	81335-37-7	50356	HBSL	NA	2,000	--	Furlong and others, 2001.
Imazethapyr	SH2060	81335-77-5	50407	HBSL	NA	20,000	--	Furlong and others, 2001.
Linuron	SH2060	330-55-2	38478	HBSL	NA	5	--	Furlong and others, 2001.
(4-Chloro-2-methylphenoxy)-acetic acid (MCPA)	SH2060	94-81-5	38482	HBSL	NA	30	--	Furlong and others, 2001.
4-(2-methyl-4-chlorophenoxy) butyric acid	SH2060	94-81-5	38487	HBSL	NA	30	--	Furlong and others, 2001.
Metolachlor	SH2003/2033	51218-45-2	39415	HBSL	CCL3	700	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
Metribuzin	SH2003/2033	21087-64-9	82630	HBSL	NA	90	--	Zaugg and others, 1995.
Metsulfuron methyl	SH2060	74223-64-6	61697	HBSL	NA	2,000	--	Furlong and others, 2001.
Molinate	SH2033	2212-67-1	82671	HBSL	CCL3	0.7	--	Zaugg and others, 1995.
Neburon	SH2060	555-37-3	49294	NA	NA	--	--	Furlong and others, 2001.
Nicosulfuron	SH2060	111991-09-4	50364	HBSL	NA	9,000	--	Furlong and others, 2001.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Tocalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Herbicides and herbicide degradates (n=68)—Continued								
Norflurazon	SH2060	27314-13-2	49293	HBSL	NA	10	--	Furlong and others, 2001.
Oryzalin	SH2060	19044-88-3	49292	HBSL	NA	4-400	--	Furlong and others, 2001.
Oxyfluorfen	SH2033	42874-03-3	61600	HBSL	CCL3	20	--	Sandstrom and others, 2001.
Pendimethalin	SH2003/2033	40487-42-1	82683	HBSL	NA	20	--	Zaugg and others, 1995.
Picloram	SH2060	1918-02-1	49291	MCL	NA	500	--	Furlong and others, 2001.
Prometon	SH2003/2033	1610-18-0	04037	HBSL	NA	400	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
Prometryn	SH2003/2033	7287-19-6	04036	HBSL	NA	300	--	Sandstrom and others, 2001.
Propanil	SH2033	709-98-8	82679	HBSL	NA	6	--	Zaugg and others, 1995.
Propham	SH2060	122-42-9	49236	HBSL	NA	100	--	Furlong and others, 2001.
Propyzamide	SH2003/2033	23950-58-5	82676	HBSL	NA	1-100	--	Zaugg and others, 1995.
Siduron	SH2060	1982-49-6	38548	HBSL	NA	1,000	--	Furlong and others, 2001.
Simazine	SH2003/2033	122-34-9	04035	MCL	NA	4	--	Zaugg and others, 1995.
Sulfometuron-methyl	SH2060	74222-97-2	50337	HBSL	NA	2,000	--	Furlong and others, 2001.
Tebuthiuron	SH2060/2033	34014-18-1	82670	HBSL	NA	1,000	--	Furlong and others, 2001.
Terbacil	SH2060	5902-51-2	04032	HBSL	NA	100	--	Furlong and others, 2001.
Terbutylazine	SH2003/2033	5915-41-3	04022	HBSL	NA	2	--	Sandstrom and others, 2001.
Thiobencarb	SH2033	28249-77-6	82681	HBSL	NA	70	--	Zaugg and others, 1995.
Triclopyr	SH2060	55335-06-3	49235	HBSL	NA	400	--	Furlong and others, 2001.
Trifluralin	SH2003/2033	1582-09-8	82661	HBSL	NA	20	--	Zaugg and others, 1995.
Insecticides and insecticide degradates (n=57)								
1-Naphthol	SH2003/2033	90-15-3	49295	NA	NA	--	Herbicide (napropamide) and insecticide (carbaryl) degradate	Sandstrom and others, 2001.
3-Hydroxycarbofuran	SH2060	16655-82-6	49308	NA	CCL3	--	Insecticide (carbofuran) degradate	Furlong and others, 2001.
Aldicarb	SH2060	1116-06-3	49312	HBSL	NA	7	--	Furlong and others, 2001.

**Appendix 1.** Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Tocalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Insecticides and insecticide degradates (n=57)—Continued								
Aldicarb sulfone	SH2060	1646–88–4	49313	HBSL	NA	7	Insecticide (aldicarb) degradate	Furlong and others, 2001.
Aldicarb sulfoxide	SH2060	1646–87–3	49314	HBSL	NA	7	Insecticide (aldicarb) degradate	Furlong and others, 2001.
<i>alpha</i> -Endosulfan	SH2033	959–98–8	34362	HBSL	NA	40	--	Sandstrom and others, 2001.
Azinphos-methyl	SH2003/2033	86–50–0	82686	HBSL	NA	10	--	Zaugg and others, 1995.
Azinphos-methyl-oxon	SH2003/2033	961–22–8	61635	NA	NA	--	Insecticide (azinphos-methyl) degradate	Sandstrom and others, 2001.
Bendiocarb	SH2060	22781–23–3	50299	HBSL	NA	9	--	Furlong and others, 2001.
Carbaryl	SH2060/2033	63–25–2	49310/ 82680	HBSL	NA	40–4,000	--	Furlong and others, 2001; Glassmeyer and others, 2005.
Carbofuran	SH2060/2033	1563–66–2	49309/ 82674	MCL	NA	40	--	Furlong and others, 2001; Zaugg and others, 1995.
Chlorpyrifos	SH2003/2033	2921–88–2	38933	HBSL	NA	2	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
Chlorpyrifos, oxygen analog	SH2003/2033	5598–15–2	61636	HBSL	NA	0.8	Insecticide (chlorpyrifos) degradate	Sandstrom and others, 2001.
<i>cis</i> -Permethrin	SH2003/2033	54774–45–7	82687	HBSL	NA	4–400	--	Zaugg and others, 1995.
Cyfluthrin	SH2003/2033	68359–37–5	61585	HBSL	NA	200	--	Sandstrom and others, 2001.
Cypermethrin	SH2003/2033	52315–07–8	61586	HBSL	NA	40	--	Sandstrom and others, 2001.
Desulfinylfipronil	SH2003/2033	--	62170	NA	NA	--	Insecticide (fipronil) degradate	Madsen and others, 2003.
Desulfinylfipronil amide	SH2003/2033	--	62169	NA	NA	--	Insecticide (fipronil) degradate	Madsen and others, 2003.
Diazinon	SH2003/2033	333–41–5	39572	HBSL	NA	1	--	Zaugg and others, 1995; Sandstrom and others, 2001; Glassmeyer and others, 2005.
Diazinon, oxygen analog	SH2003/2033	962–58–3	61638	NA	NA	--	Insecticide (diazinon) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Tocalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Insecticides and insecticide degradates (n=57)—Continued								
Dichlorvos	SH2003/2033	62-73-7	38775	HBSL	NA	0.4	--	Zaugg and others, 1995; Sandstrom and others, 2001; Glassmeyer and others, 2005.
Dicrotophos	SH2003/2033	141-66-2	38454	HBSL	CCL3	0.05	--	Zaugg and others, 1995; Sandstrom and others, 2001.
Dieldrin	SH2003/2033	60-57-1	39381	HBSL	NA	0.002-0.2	--	Zaugg and others, 1995; Sandstrom and others, 2001.
Dimethoate	SH2003/2033	60-51-5	82662	HBSL	CCL3	2	--	Zaugg and others, 1995; Sandstrom and others, 2001.
Disulfoton	SH2033	298-04-4	82677	HBSL	CCL3	0.9	--	Zaugg and others, 1995.
Disulfoton sulfone	SH2033	2497-06-5	61640	NA	NA	--	Insecticide (disulfoton) degradate	Sandstrom and others, 2001.
Endosulfan sulfate	SH2033	1031-07-8	61590	NA	NA	--	Insecticide ( <i>alpha</i> -endosulfan) degradate	Sandstrom and others, 2001.
Ethion	SH2003/2033	563-12-2	82346	HBSL	NA	4	--	Zaugg and others, 1995; Sandstrom and others, 2001.
Ethion monooxon	SH2003/2033	17356-42-2	61644	NA	NA	--	Insecticide (ethion) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.
Ethoprophos	SH2033	13194-48-4	82672	HBSL	CCL3	1-100	--	Zaugg and others, 1995.
Fenamiphos	SH2003/2033	22224-92-6	61591	HBSL	CCL3	0.7	--	Zaugg and others, 1995; Sandstrom and others, 2001.
Fenamiphos sulfone	SH2003/2033	31972-44-8	61645	NA	NA	--	Insecticide (fenamiphos) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.
Fenamiphos sulfoxide	SH2003/2033	31972-43-7	61646	NA	NA	--	Insecticide (fenamiphos) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.
Fipronil	SH2003/2033	120068-37-3	62166	HBSL	NA	0.1	--	Madsen and others, 2003.

**Appendix 1.** Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Insecticides and insecticide degradates (n=57)—Continued								
Fipronil sulfide	SH2003/2033	120067-83-6	62167	NA	NA	--	Insecticide (fipronil) degradate	Madsen and others, 2003.
Fipronil sulfone	SH2003/2033	120068-36-2	62168	NA	NA	--	Insecticide (fipronil) degradate	Madsen and others, 2003.
Fonofos	SH2003/2033	944-22-9	04095	HBSL	NA	10	--	Zaugg and others, 1995.
Imidacloprid	SH2060	138261-41-3	61695	NA	NA	--	--	Furlong and others, 2001.
Isofenphos	SH2003/2033	25311-71-1	61594	HBSL	NA	6	--	Sandstrom and others, 2001.
<i>lambda</i> -Cyhalothrin	SH2033	91465-08-6	61595	HBSL	NA	7	--	Wood, 2010.
Malaoxon	SH2003/2033	1634-78-2	61652	NA	NA	--	Insecticide (malathion) degradate	Sandstrom and others, 2001.
Malathion	SH2003/2033	121-75-5	39532	HBSL	NA	500	--	Zaugg and others, 1995.
Methidathion	SH2003/2033	950-37-8	61598	HBSL	NA	1	--	Sandstrom and others, 2001.
Methiocarb	SH2060	2032-65-7	38501	HBSL	NA	40	--	Furlong and others, 2001.
Methomyl	SH2060	16752-77-5	49296	HBSL	NA	200	--	Furlong and others, 2001.
Oxamyl	SH2060	23135-22-0	38866	MCL	NA	200	--	Furlong and others, 2001.
Paraoxon-methyl	SH2003/2033	950-35-6	61664	NA	NA	--	Insecticide (methyl parathion) degradate	Sandstrom and others, 2001.
Parathion-methyl	SH2003/2033	298-00-0	82667	HBSL	NA	1	--	Zaugg and others, 1995.
Phorate	SH2003/2033	298-02-2	82664	HBSL	NA	4	--	Zaugg and others, 1995.
Phorate oxon	SH2003/2033	2600-69-3	61666	NA	NA	--	Insecticide (phorate) degradate	Sandstrom and others, 2001.
Phosmet	SH2003/2033	732-11-6	61601	HBSL	NA	4	--	Sandstrom and others, 2001.
Phosmet oxon	SH2003/2033	3735-33-9	61668	NA	NA	--	Insecticide (phosmet) degradate	Sandstrom and others, 2001.
Propargite	SH2033	2312-35-8	82685	HBSL	NA	1-100	--	Zaugg and others, 1995.
Propoxur	SH2060	114-26-1	38538	NAV	NA	NAV	--	Furlong and others, 2001.
Tefluthrin	SH2033	79538-32-2	61606	HBSL	NA	40	--	Sandstrom and others, 2001.
Terbufos	SH2003/2033	13071-79-9	82675	HBSL	CCL3	0.4	--	Zaugg and others, 1995.
Terbufos oxygen analog sulfone	SH2003/2033	56070-15-6	61674	NA	NA	--	Insecticide (terbufos) degradate	Sandstrom and others, 2001.



**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Manufacturing additives (n=6)								
5-Methyl-1 <i>H</i> -benzotriazole	SH1433	136-85-6	62063	NA	NA	--	Corrosion inhibitor in de-icers/antifreeze, anti-fading agent for metals, antiseptic and anticoagulant agent, anti-fog for photography, ultraviolet-absorbers, photoconductor, copying systems, pharmaceuticals, pesticide products and other specialty chemicals, antioxidant	Zaugg and others, 2002; Glassmeyer and others, 2005; Chemicaland21, 2010.
Tri(2-butoxyethyl) phosphate	SH1433	78-51-3	62093	NA	NA	--	Plasticizer, pesticide adjuvant, flame retardant	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. Environmental Protection Agency, 2009c.
Tri(2-chloroethyl) phosphate	SH1433	115-96-8	62087	NA	NA	--	Flame retardant, fire resistant cellulose plasticizer	Zaugg and others, 2002; Glassmeyer and others, 2005.
Tributyl phosphate	SH1433	126-73-8	62089	NA	NA	--	Antifoaming agent and flame retardant	Zaugg and others, 2002.
Triphenyl phosphate	SH1433	115-86-6	62092	NA	NA	--	Plasticizer, flame retardant	Budavari, 1989; Zaugg and others, 2002; Glassmeyer and others, 2005.
Tris(dichloroisopropyl) phosphate	SH1433	13674-87-8	62088	NA	NA	--	Flame retardant, plasticizer	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
Organic synthesis compounds (n=18)								
1,1-Dichloropropene	SH2020	563-58-6	77168	NA	NA	--	Solvent (pharmaceuticals)	Bender and others, 1999; Scorecard, 2006.
1,2,3-Trichlorobenzene	SH2020	87-61-6	77613	NA	NA	--	Termiticide, solvent	Budavari, 1989, 1996; Bender and others, 1999; U.S. National Library of Medicine, 2006.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
1,2,3-Trichloropropane	SH2020	96–18–4	77443	NA	CCL3	NAV	Fumigant contaminant, paint and varnish remover	Agency for Toxic Substances and Disease Registry, 1992a; Tesoriero and others, 2001.
3-Chloro-1-propene	SH2020	107–05–1	78109	NA	NA	--	Fumigant contaminant	Cohen and others, 1983; U.S. National Library of Medicine, 2006.
Acrylonitrile	SH2020	107–13–1	34215	HBSL	NA	0.06–6	Fumigant, pesticide	Bender and others, 1999; Scorecard, 2006.
Anthraquinone	SH1433	84–65–1	62066	NA	NA	--	Bird repellent, serves as the basis for the production of a large number of acid and base dyes, vat dyes, disperse dyes, and reactive dyes additive in the soda and kraft chemical alkaline pulping processes in the paper pulping industry	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. National Library of Medicine, 2006.
Carbazole	SH1433	86–74–8	62071	NA	NA	--	Synthesis of dyes, combustion product	Budavari, 1989; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
Carbon disulfide	SH2020	75–15–0	77041	HBSL	NA	700	Solvent, syntheses, fumigant, sulfate-reduction product	Budavari, 1989; Megonigal and others, 2004; Scorecard, 2006.
Chloromethane	SH2020	74–87–3	34418	NAV	CCL3	NAV	Blowing agent/propellant, solvent, refrigerant	Budavari, 1989; U.S. National Library of Medicine, 2006.
Ethyl methacrylate (ethyl 2-methyl-2-propanoate)	SH2020	97–63–2	73570	NA	NA	--	Hairspray, used to make polymers, chemical intermediate	Scorecard, 2006; U.S. National Library of Medicine, 2006.
Hexachlorobutadiene	SH2020	87–68–3	39702	HBSL	NA	0.9–90	Used in rubber manufacture, solvent, pesticide (non-U.S.)	Bender and others, 1999; California Environmental Protection Agency, 1999.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Organic synthesis compounds (n=18)—Continued								
Iodomethane	SH2020	74–88–4	77424	NA	NA	--	Microscopy, circuit board manufacture, fire extinguishers, proposed fumigant	Budavari, 1989; U.S. Environmental Protection Agency, 2006b.
Methyl acrylate (methyl-2-propenoate)	SH2020	96–33–3	49991	NA	NA	--	Manufacture of resins, paper, plastic	Budavari, 1989; U.S. National Library of Medicine, 2006.
Methyl acrylonitrile (2-methyl-2-propenenitrile)	SH2020	126–98–7	81593	HBSL	NA	0.7	Organic synthesis, polymer manufacture, chemical intermediate	Budavari, 1989; United Nations Environmental Programme, 2002; U.S. National Library of Medicine, 2006.
Methyl methacrylate (methyl 2-methyl-2-propenoate)	SH2020	80–62–6	81597	HBSL	NA	10,000	Manufacture of paint, paper, acrylic, chemical intermediate, pesticide adjuvant	U.S. National Library of Medicine, 2006; U.S. Environmental Protection Agency, 2009c; Spectrum Laboratories Inc., 2010a.
<i>trans</i> -1,4-Dichloro-2-butene	SH2020	110–57–6	73547	NA	NA	--	Chemical intermediate	U.S. National Library of Medicine, 2006.
Vinyl bromide	SH2020	593–60–2	50002	NA	NA	--	Plastic manufacture, 1,2-dibromoethane degradate, flame retardant	Barbush and Reinhard, 1989; Bender and others, 1999.
Vinyl chloride	SH2020	75–01–4	39175	MCL	NA	2	Polyvinyl chloride (PVC) manufacture, refrigerant, degradate of 1,2-dichloroethane (aerobic) and dichloroethylene (anaerobic)	Vogel and McCarty, 1985; Barbash and Reinhard, 1989; Bender and others, 1999.
Pavement- and combustion-derived compounds (n=5)								
Anthracene	SH1433	120–12–7	34221	HBSL	NA	2,000	Polynuclear aromatic hydrocarbon, used in dye production and production of plastic fibers, organic synthesis (anthraquinone), wood preservative	Lee and Strahan, 2003; Glassmeyer and others, 2005.
Benzo[ <i>a</i> ]pyrene	SH1433	50–32–8	34248	MCL	NA	0.2	Polynuclear aromatic hydrocarbon, cancer research chemical	Zaugg and others, 2002; Glassmeyer and others, 2005.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Pavement- and combustion-derived compounds (n=5)—Continued								
Fluoranthene	SH1433	206-44-0	34377	HBSL	NA	300	Polynuclear aromatic hydrocarbon, used on inside lining on iron water pipes and tanks, production of fluorescent dyes and pharmaceuticals, component of coal tar and asphalt	Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
Phenanthrene	SH1433	85-01-8	34462	NA	NA	--	Polynuclear aromatic hydrocarbon, manufacture of dyes, explosives, and drugs, used in research	Zaugg and others, 2002; Glassmeyer and others, 2005.
Pyrene	SH1433	129-00-0	34470	HBSL	NA	200	Polynuclear aromatic hydrocarbon, used to synthesize benzo[a]pyrene, used as a starting material in the production of optical brighteners and dyes, research chemical, component of coal tar and asphalt	Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
Personal-care and domestic-use products (n=22)								
3- <i>tert</i> -Butyl-4-hydroxy anisole (BHA)	SH1433	25013-16-5	62059	NA	CCL3	--	Antioxidant, preservative, food packaging, and rubber and petroleum products	Zaugg and others, 2002; Glassmeyer and others, 2005.
4-Cumylphenol	SH1433	599-64-4	62060	NA	NA	--	Nonionic detergent metabolite	Zaugg and others, 2002; Glassmeyer and others, 2005.
4- <i>n</i> -Octylphenol	SH1433	1806-26-4	62061	NA	NA	--	Nonionic detergent metabolite	Zaugg and others, 2002; Glassmeyer and others, 2005.
4- <i>tert</i> -Octylphenol	SH1433	140-66-9	62062	NA	NA	--	Nonionic detergent metabolite	Zaugg and others, 2002; Glassmeyer and others, 2005.
Acetophenone	SH1433	98-86-2	62064	HBSL	NA	700	Fragrance, flavorant, solvent for paint and varnish removal, plastics and resins	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. National Library of Medicine, 2006.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Personal-care and domestic-use products (n=22)—Continued								
Acetyl hexamethyl tetrahydronaphthalene (AHTN)	SH1433	21145-77-7	62065	NA	NA	--	Widely used musk fragrance	Zaugg and others, 2002.
Bromochloromethane	SH2020	74-97-5	77297	HBSL	CCL3	90	Fire extinguishing fluid, intermediate in pesticide manufacturing	Bender and others, 1999; U.S. National Library of Medicine, 2006.
Caffeine	SH2060	58-08-2	50305	NA	NA	--	Beverage ingredient, diuretic	Furlong and others, 2001; Glassmeyer and others, 2005.
Camphor	SH1433	76-22-2	62070	NA	NA	--	Flavorant and odorant, used in manufacture of plastics, as plasticizer for cellulose esters and ethers, in lacquers and varnishes, in explosives, in pyrotechnics, in embalming fluid, in manufacture of cymene, in camphorated parachlorophenol, paregoric, and flexible collodion	Budavari, 1989; Zaugg and others, 2002; U.S. National Library of Medicine, 2005.
Cotinine	SH1433	486-56-6	62005	NA	NA	--	Primary nicotine metabolite, non-prescription drug	Kolpin and others, 2002; Zaugg and others, 2002; Glassmeyer and others, 2005.
<i>d</i> -Limonene	SH1433	5989-27-5	62073	NA	NA	--	Antimicrobial, fragrance	Zaugg and others, 2002; Glassmeyer and others, 2005.
Hexahydrohexamethylcyclopentabenzopyran (HHCB)	SH1433	1222-05-5	62075	NA	NA	--	Widely used musk fragrance	Zaugg and others, 2002; Glassmeyer and others, 2005.
Indole	SH1433	120-72-9	62076	NA	NA	--	Pesticide adjuvant, coffee ingredient, fragrance	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
Isoborneol	SH1433	124-76-5	62077	NA	NA	--	Flavorant, fragrance, disinfection ingredient	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. National Library of Medicine, 2006.

**Appendix 1.** Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.—Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Personal-care and domestic-use products (n=22)—Continued								
Isoquinoline	SH1433	119-65-3	62079	NA	NA	--	Flavors and fragrances	Zaugg and others, 2002; Glassmeyer and others, 2005.
Menthol (5-methyl-2-[1-methylethyl]cyclohexanol)	SH1433	89-78-1	62080	HBSL	NA	10,000	Cigarettes, cough drops, linament, mouthwash	Zaugg and others, 2002.
Methyl salicylate	SH1433	119-36-8	62081	NAV	NA	NAV	Analgesic, decongestant, toilet and window cleaner	Kolpin and others, 2002; Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006.
Nonylphenol, diethoxy-(total)	SH1433	26027-38-2	62083	NA	NA	--	Nonionic detergent metabolite	Zaugg and others, 2002.
Octylphenol, diethoxy-(OPEO2)	SH1433	--	61705	NA	NA	--	Nonionic detergent metabolite	Zaugg and others, 2002.
Octylphenol, monoethoxy-(OPEO1)	SH1433	--	61706	NA	NA	--	Nonionic detergent metabolite	Zaugg and others, 2002.
Triclosan	SH1433	3380-34-5	62090	HBSL	NA	2,000	Antimicrobial, preservative for cosmetics and detergents preparations	Zaugg and others, 2002; Glassmeyer and others, 2005.
Triethyl citrate	SH1433	77-93-0	62091	NA	NA	--	Cosmetics, pharmaceuticals, plasticizer	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
Plant- or animal-derived biochemicals (n=5)								
3-beta-Coprostanol	SH1433	360-68-9	62057	NA	NA	--	Fecal indicator (carnivores)	Zaugg and others, 2002; Glassmeyer and others, 2005.
3-Methyl-1( <i>H</i> )-indole (Skatole)	SH1433	83-34-1	62058	NA	NA	--	In animal waste, stench in feces, in coal tar	Zaugg and others, 2002; Glassmeyer and others, 2005.
beta-Sitosterol	SH1433	83-46-5	62068	NA	NA	--	Plant sterol	Zaugg and others, 2002; Glassmeyer and others, 2005.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number; HHB, human-health benchmark; CCL, Contaminant Candidate List (U.S. Environmental Protection Agency, 2012a); µg/L, micrograms per liter; n, number of study locations; SH, laboratory schedule that lists compounds and analytical method; MCL, Maximum Contaminant Level (U.S. Environmental Protection Agency, 2006a); NA, not applicable; --, no information available; HBSL, U.S. Geological Survey Health-Based Screening Level (Toccalino and others, 2008); CCL3, a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations, that are known or anticipated to occur in public water systems, and which may require regulation under the Safe Drinking Water Act; NAV, not available; LCPD, Acetamide Pesticide Method (Lee and Strahan, 2003)]

Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Plant- or animal-derived biochemicals (n=5)—Continued								
<i>beta</i> -Stigmastanol	SH1433	19466–47–8	62086	NA	NA	--	Plant sterol	Zaugg and others, 2002; Glassmeyer and others, 2005.
Cholesterol	SH1433	57–88–5	62072	NA	NA	--	Fecal indicator, plant sterol	Zaugg and others, 2002; Glassmeyer and others, 2005.
Refrigerants and propellants (n=3)								
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	SH2020	76–13–1	77652	HBSL	NA	200,000	Electroplating, degreasing, adhesives, textiles, pesticide adjuvant	Bender and others, 1999; CambridgeSoft Corporation, 2010; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
Dichlorodifluoromethane (CFC-12)	SH2020	75–71–8	34668	HBSL	NA	1,000	Insulation, inhalers, insecticide, pesticide adjuvant	Bender and others, 1999; CambridgeSoft Corporation, 2010; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
Trichlorofluoromethane (CFC-11)	SH2020	75–69–4	34488	HBSL	NA	2,000	Hairspray, inhalers, insecticide, pesticide adjuvant	Bender and others, 1999; CambridgeSoft Corporation, 2010; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
Solvents (n=32)								
1,1,1,2-Tetrachloroethane	SH2020	630–20–6	77562	HBSL	CCL3	70	Solvent for varnish	Bender and others, 1999; Scorecard, 2006.
1,1,1-Trichloroethane	SH2020	71–55–6	34506	MCL	NA	200	Electronics, pharmaceutical manufacture, degreaser, pesticide adjuvant, fumigant	Bender and others, 1999; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
1,1,2,2-Tetrachloroethane	SH2020	79–34–5	34516	HBSL	NA	0.2–20	Manufacture of solvents, insecticide, pesticide adjuvant	Bender and others, 1999; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
1,1,2-Trichloroethane	SH2020	79–00–5	34511	MCL	NA	5	Aerosol paints, manufacture solvent	Bender and others, 1999; Scorecard, 2006.

**Appendix 1.** Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.—Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Solvents (n=32)—Continued								
1,1-Dichloroethane	SH2020	75–34–3	34496	NA	CCL3	--	Lubricant, cleaner; anaerobic 1,1,1-trichloroethane degradate	Klecka and others, 1990; Bender and others, 1999; Scorecard, 2006.
1,1-Dichloroethene	SH2020	75–35–4	34501	MCL	NA	7	1,1,1-trichloroethane degradate (aerobic); pharmaceutical solvent	Haag and Mill, 1988; Bender and others, 1999; Scorecard, 2006.
1,2,4-Trichlorobenzene	SH2020	120–82–1	34551	MCL	NA	70	Manufacture of solvents; insecticide	Bender and others, 1999; Scorecard, 2006.
1,2-Dichlorobenzene (o-dichlorobenzene)	SH2020	95–50–1	34536	MCL	NA	600	Disinfectant, deodorant, consumer solvent	Bender and others, 1999; Scorecard, 2006.
1,2-Dichloroethane (ethylene dichloride)	SH2020	107–06–2	32103	MCL	NA	5	Fumigant, manufacture of solvents, anti-knock compound in gasoline	Bender and others, 1999; National Oceanic and Atmospheric Administration, 2008; Scorecard, 2006.
1,3-Dichlorobenzene (m-dichlorobenzene)	SH2020	541–73–1	34566	HBSL	NA	600	Organic synthesis, fumigant	Bender and others, 1999.
2-Chlorotoluene	SH2020	95–49–8	77275	HBSL	NA	100	Pesticide adjuvant	Bender and others, 1999; U.S. Environmental Protection Agency, 2009c.
2-Hexanone	SH2020	591–78–6	77103	HBSL	NA	40	Organic synthesis	Agency for Toxic Substances and Disease Registry, 1992b; Spectrum Laboratories Inc., 2010b.
4-Chlorotoluene	SH2020	106–43–4	77277	HBSL	NA	100	Pesticide adjuvant	Bender and others, 1999; U.S. Environmental Protection Agency, 2009c.
Acetone (2-propanone)	SH2020	67–64–1	81552	HBSL	NA	6,000	Organic synthesis, chemical intermediate, pesticide adjuvant	Budavari, 1989; U.S. Environmental Protection Agency, 2009c.
Bromobenzene	SH2020	108–86–1	81555	HBSL	NA	60	Organic synthesis, additive to oil	Bender and others, 1999; U.S. National Library of Medicine, 2006.
Carbon tetrachloride	SH2020	56–23–5	32102	MCL	NA	5	Fumigant, solvent	Bender and others, 1999; Scorecard, 2006.
Chlorobenzene	SH2020	108–90–7	34301	MCL	NA	100	Disinfectant, herbicide, building materials, solvent	Budavari, 1989; Bender and others, 1999; Scorecard, 2006.



**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Chloroethane	SH2020	75-00-3	34311	NA	NA	--	Refrigerant, anaerobic degradation of 1,1,1-trichloroethane and 1,1-dichloroethane, manufacture of tetraethyl lead	Klecka and others, 1990; Bender and others, 1999; Lorah and Olsen, 1999.
<i>cis</i> -1,2-Dichloroethene	SH2020	156-59-2	77093	MCL	NA	70	Trichloroethene degradate (anaerobic)	Bender and others, 1999; Lorah and Olsen, 1999.
Dibromomethane	SH2020	74-95-3	30217	NA	NA	--	Organic synthesis (pesticide manufacture), heavy liquid for mineral separations, fire extinguishers	Bender and others, 1999.
Diethyl ether (1,1'-oxybisethane)	SH2020	60-29-7	81576	HBSL	NA	1,000	Detergent, solvent, pharmaceuticals, cosmetics	Budavari, 1989; Scorecard, 2006.
Hexachloroethane	SH2020	67-72-1	34396	HBSL	NA	0.7	Lubricant, dry cleaning solvent	Budavari, 1989; Scorecard, 2006.
Methyl acetate	SH4024	79-20-9	77032	NA	NA	--	Aerosol paints	Scorecard, 2006.
Methyl ethyl ketone (MEK)	SH2020	78-93-3	81595	HBSL	NA	4,000	Adjuvant, solvent, cleaners, polyvinyl chloride (PVC) glue and primer	Bender and others, 1999; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
Methyl isobutyl ketone (MIBK) (4-methyl-2-pentanone)	SH2020	108-10-1	78133	NA	NA	--	Solvent, personal care products, insecticide, pesticide adjuvant, polyvinyl chloride (PVC) glue	Budavari, 1989; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
Methylene chloride	SH2020	75-09-2	34423	MCL	NA	5	Solvent, personal care products, insecticide, rodenticide, fumigant, dog repellent, anaerobic degradation of carbon tetrachloride, polyvinyl chloride (PVC) glue substitute	Egli and others, 1988; Bender and others, 1999; Scorecard, 2006.
<i>n</i> -Propylbenzene	SH2020	103-65-1	77224	NA	CCL3	--	Insulation, flooring manufacture	Bender and others, 1999; Scorecard, 2006.
<i>p</i> -Cresol	SH1433	106-44-5	62084	NA	NA	--	Paint/varnish removal, solvent, disinfectant, chemical intermediate for synthetic resins	Budavari, 1989; Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006.

**Appendix 1.** Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.—Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Solvents (n=32)—Continued								
Perchloroethene (PCE); tetrachloroethene)	SH2020	127–18–4	34475	MCL	NA	5	Fumigant, solvent	Bender and others, 1999; Glassmeyer and others, 2005; Scorecard, 2006.
Tetrahydrofuran (1,4-epoxybutane)	SH2020	109–99–9	81607	NA	NA	--	Adjuvant, cleaners, solvent, polyvinyl chloride (PVC) glue and primer	Budavari, 1989; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c.
<i>trans</i> -1,2-Dichloroethene	SH2020	156–60–5	34546	MCL	NA	100	Trichloroethene degradate	Bender and others, 1999; Lorah and Olsen, 1999.
Trichloroethene (TCE)	SH2020	79–01–6	39180	MCL	NA	5	Fumigant, solvent, anaerobic per-chloroethene degradate	Vogel and McCarty, 1985; Bender and others, 1999; Scorecard, 2006.
Compounds removed from dataset (n=11)								
3-Ketocarbofuran	SH2060	16709–30–1	50295	NA	NA	--	Insecticide (carbofuran) degradate	Furlong and others, 2001.
Benzophenone	SH1433	119–61–9	62067	NA	NA	--	Fixative in perfumes and soaps, hair mousse, inks, organic synthesis	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. National Library of Medicine, 2006.
Bisphenol A	SH1433	80–05–7	62069	HBSL	NA	400	Used in manufacture of plastic and polycarbonate resins	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
Chlorothalonil	SH2060	1897–45–6	49306	HBSL	NA	5–500	--	Furlong and others, 2001.
Deethyldeisopropyl-atrazine	SH2060	3397–62–4	04039	NA	NA	--	Herbicide (atrazine) degradate	Furlong and others, 2001.
Fonofos, oxygen analog	SH2003	944–21–8	61649	NA	NA	--	Insecticide (fonofos) degradate	Sandstrom and others, 2001.
Isophorone	SH1433	78–59–1	34409	HBSL	NA	100	Herbicide, adjuvant, solvent	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009c; U.S. National Library of Medicine, 2006.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—  
Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Compounds removed from dataset (n=11)—Continued								
<i>N,N</i> -diethyl- <i>meta</i> -toluamide (DEET)	SH1433	134-62-3	62082	NA	NA	--	Insect repellent	Zaugg and others, 2002; Glassmeyer and others, 2005.
<i>para</i> -Nonylphenol (total)	SH1433	84852-15-3	62085	NA	NA	--	Surfactant intermediate	Zaugg and others, 2002; Glassmeyer and others, 2005.
Pentachlorophenol	SH1433	87-86-5	34459	MCL	NA	1	Wood preservative, herbicide, insecticide, plant growth regulator	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; Wood, 2010.
Phenol	SH1433	108-95-2	34466	HBSL	NA	2,000	Disinfectant	Zaugg and others, 2002; Glassmeyer and others, 2005.
Additional herbicide and herbicide degradates analyzed (n=19)								
Acetochlor ethane sulfonic acid	LCPD	187022-11-3	61029	NA	CCL3	--	Herbicide (acetochlor) degradate	Lee and Strahan, 2003.
Acetochlor oxanilic acid	LCPD	184992-44-4	61030	NA	CCL3	--	Herbicide (acetochlor) degradate	Lee and Strahan, 2003.
Acetochlor sulfynilacetic acid	LCPD	--	62847	NA	NA	--	Herbicide (acetochlor) degradate	Lee and Strahan, 2003.
Acetochlor/metolachlor ethane sulfonic acid 2nd amide	LCPD	--	62850	NA	NA	--	Herbicide (acetochlor or metolachlor) degradate	Lee and Strahan, 2003.
Alachlor ethane sulfonic acid	LCPD	142363-53-9	50009	NA	CCL3	--	Herbicide (alachlor) degradate	Lee and Strahan, 2003.
Alachlor ethane sulfonic acid 2nd amide	LCPD	--	62849	NA	NA	--	Herbicide (alachlor) degradate	Lee and Strahan, 2003.
Alachlor oxanilic acid	LCPD	171262-17-2	61031	NA	CCL3	--	Herbicide (alachlor) degradate	Lee and Strahan, 2003.
Alachlor sulfynilacetic acid	LCPD	140939-16-8	62848	NA	NA	--	Herbicide (alachlor) degradate	Lee and Strahan, 2003.

**Appendix 1. Compounds monitored, Chemical Abstract Service Registry number (CASRN), drinking-water benchmark, primary use or source group, and analytical schedule.**—Continued

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Compound name	USGS schedule	CASRN <sup>a</sup>	USGS parameter code	HHB	CCL	Benchmark value (µg/L)	Compound use or source	Reference
Additional herbicide and herbicide degradates analyzed (n=19)—Continued								
Dimethenamid	LCPD	87674-68-8	61588	NA	NA	--	--	Lee and Strahan, 2003.
Dimethenamid ethane sulfonic acid	LCPD	205939-58-8	61951	NA	NA	--	Herbicide (dimethenamid) degrade	Lee and Strahan, 2003.
Dimethenamid oxanilic acid	LCPD	--	62482	NA	NA	--	Herbicide (dimethenamid) degrade	Lee and Strahan, 2003.
Flufenacet	LCPD	142459-58-3	62481	NA	NA	--	--	Lee and Strahan, 2003.
Flufenacet ethane sulfonic acid	LCPD	--	61952	NA	NA	--	Herbicide (flufenacet) degrade	Lee and Strahan, 2003.
Flufenacet oxanilic acid	LCPD	--	62483	NA	NA	--	Herbicide (flufenacet) degrade	Lee and Strahan, 2003.
Metolachlor ethane sulfonic acid	LCPD	171118-09-5	61043	NA	CCL3	--	Herbicide (metolachlor) degrade	Lee and Strahan, 2003.
Metolachlor oxanilic acid	LCPD	152019-73-3	61044	NA	CCL3	--	Herbicide (metolachlor) degrade	Lee and Strahan, 2003.
Propachlor	LCPD	1918-16-7	04024	HBSL	NA	1-100	--	Lee and Strahan, 2003.
Propachlor ethane sulfonic acid	LCPD	--	62766	NA	NA	--	Herbicide (propachlor) degrade	Lee and Strahan, 2003.
Propachlor oxanilic acid	LCPD	--	62767	NA	NA	--	Herbicide (propachlor) degrade	Lee and Strahan, 2003.

<sup>a</sup>This report contains Chemical Abstracts Service Registry Numbers (CASRN)<sup>®</sup>, which is a Registered Trademark of the American Chemical Society. The CASRN online database provides the latest registry number information: <http://www.cas.org/>. Chemical Abstracts Service recommends the verification of the CASRNs through CAS Client Services<sup>SM</sup>.

<sup>b</sup>The MCL of 80 µg/L is for the sum of the concentrations of the four disinfection by-products: bromodichloromethane, bromoform, chloroform, dibromochloromethane.

<sup>c</sup>Letter prefix added to CASRN not available for *cis*- and *trans*-isomers.

<sup>d</sup>The concentrations of *m*- & *p*-xylene and *o*-xylene are compared to the MCL of 10,000 µg/L for mixed xylenes, CASRN 1330-20-7.

## **Appendix 2. Summary of the Frequency of Detections in Surface-Water Samples**

**Appendix 2. Summary of the frequency of detections in surface-water samples.**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Disinfection by-products									
Chloroform	67-66-3	SH2020	300	189	63.00	82	27.33	46	15.33
Bromodichloromethane	75-27-4	SH2020	300	51	17.00	28	9.33	10	3.33
Dibromochloromethane	124-48-1	SH2020	300	7	2.33	7	2.33	2	0.67
Bromoform	75-25-2	SH2020	300	3	1.00	3	1.00	0	0.00
Fumigant-related compounds									
1,4-Dichlorobenzene ( <i>p</i> -dichlorobenzene)	106-46-7	SH2020	300	25	8.33	3	1.00	0	0.00
1,2-Dichloropropane	78-87-5	SH2020	300	2	0.67	0	0.00	0	0.00
1,2-Dibromo-3-chloropropane (DBCP)	96-12-8	SH2020	300	0	0.00	0	0.00	0	0.00
1,2-Dibromoethane (EDB)	106-93-4	SH2020	300	0	0.00	0	0.00	0	0.00
1,3-Dichloropropane	142-28-9	SH2020	300	0	0.00	0	0.00	0	0.00
2,2-Dichloropropane	594-20-7	SH2020	300	0	0.00	0	0.00	0	0.00
Bromomethane (methyl bromide)	74-83-9	SH2020	300	0	0.00	0	0.00	0	0.00
<i>cis</i> -1,3-Dichloropropene	10061-01-5	SH2020	300	0	0.00	0	0.00	0	0.00
<i>trans</i> -1,3-Dichloropropene	10061-02-6	SH2020	300	0	0.00	0	0.00	0	0.00
Fungicides and fungicide degradates									
Benomyl	17804-35-2	SH2060	283	25	8.83	3	1.06	1	0.35
Iprodione	36734-19-7	SH2003/2033	302	6	1.99	2	0.66	1	0.33
<i>trans</i> -Propiconazole	t-60207-90-1 <sup>b</sup>	SH2033	128	9	7.03	0	0.00	0	0.00
<i>cis</i> -Propiconazole	c-60207-90-1 <sup>b</sup>	SH2033	128	8	6.25	0	0.00	0	0.00
Metalaxyl	57837-19-1	SH2003/2033	302	17	5.63	0	0.00	0	0.00
Myclobutanil	88671-89-0	SH2003/2033	302	6	1.99	0	0.00	0	0.00
3,5-Dichloroaniline	626-43-7	SH2033	127	2	1.57	0	0.00	0	0.00
Propiconazole	60207-90-1	SH2060	283	1	0.35	0	0.00	0	0.00
Tebuconazole	107534-96-3	SH2033	123	0	0.00	0	0.00	0	0.00
Gasoline hydrocarbons, oxygenates, and oxygenate degradates									
Methyl <i>tert</i> -butyl ether (MTBE)	1634-04-4	SH2020	301	73	24.25	63	20.93	39	12.96
Toluene	108-88-3	SH2020	216	32	14.81	31	14.35	14	6.48

## Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Gasoline hydrocarbons, oxygenates, and oxygenate degradates—Continued									
<i>m</i> - & <i>p</i> -Xylene	<i>m</i> : 108-38-3; <i>p</i> : 106-42-3	SH2020	300	47	15.67	26	8.67	14	4.67
<i>tert</i> -Butyl alcohol	75-65-0	SH4024	297	17	5.72	17	5.72	17	5.72
1,2,4-Trimethylbenzene	95-63-6	SH2020	300	30	10.00	15	5.00	5	1.67
<i>o</i> -Xylene	95-47-6	SH2020	300	29	9.67	13	4.33	7	2.33
Benzene	71-43-2	SH2020	283	95	33.57	11	3.89	6	2.12
Naphthalene	91-20-3	SH2020	300	9	3.00	9	3.00	9	3.00
<i>tert</i> -Amyl methyl ether (TAME)	994-05-8	SH2020	301	12	3.99	8	2.66	2	0.66
Ethylbenzene	100-41-4	SH2020	300	26	8.67	7	2.33	1	0.33
1-Methylnaphthalene	90-12-0	SH1433	298	11	3.69	1	0.34	0	0.00
1-Ethyl-2-methylbenzene	611-14-3	SH2020	300	14	4.67	1	0.33	1	0.33
1,3,5-Trimethylbenzene	108-67-8	SH2020	300	11	3.67	1	0.33	1	0.33
1,2,3-Trimethylbenzene	526-73-8	SH2020	300	7	2.33	1	0.33	1	0.33
1,2,3,5-Tetramethylbenzene	527-53-7	SH2020	300	3	1.00	1	0.33	0	0.00
2-Methylnaphthalene	91-57-6	SH1433	298	11	3.69	0	0.00	0	0.00
Styrene	100-42-5	SH2020	287	2	0.70	0	0.00	0	0.00
2,6-Dimethylnaphthalene	581-42-0	SH1433	298	1	0.34	0	0.00	0	0.00
Isopropylbenzene	98-82-8	SH2020	300	1	0.33	0	0.00	0	0.00
<i>n</i> -Butylbenzene	104-51-8	SH2020	300	1	0.33	0	0.00	0	0.00
Ethyl <i>tert</i> -butyl ether (ETBE)	637-92-3	SH2020	301	1	0.33	0	0.00	0	0.00
<i>tert</i> -Amyl alcohol (2-methyl-2-butanol)	75-85-4	SH4024	298	0	0.00	0	0.00	0	0.00
1,2,3,4-Tetramethylbenzene	488-23-3	SH2020	300	0	0.00	0	0.00	0	0.00
Diisopropyl ether (DIPE)	108-20-3	SH2020	301	0	0.00	0	0.00	0	0.00
<i>p</i> -Isopropyltoluene ( <i>p</i> -cymene)	99-87-6	SH2020	300	0	0.00	0	0.00	0	0.00
<i>sec</i> -Butylbenzene	135-98-8	SH2020	300	0	0.00	0	0.00	0	0.00
<i>tert</i> -Butylbenzene	98-06-6	SH2020	300	0	0.00	0	0.00	0	0.00

**Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Herbicides and herbicide degradates									
Atrazine	1912-24-9	SH2003/2033	304	212	69.74	83	27.30	63	20.72
2,4-Dichlorophenoxyacetic acid (2,4-D)	94-75-7	SH2060	284	107	37.68	58	20.42	33	11.62
Simazine	122-34-9	SH2003/2033	304	192	63.16	59	19.41	46	15.13
2-Hydroxyatrazine	2163-68-0	SH2060	280	124	44.29	53	18.93	40	14.29
Deethylatrazine	6190-65-4	SH2003/2033	304	189	62.17	56	18.42	20	6.58
Metolachlor	51218-45-2	SH2003/2033	279	163	58.42	32	11.47	18	6.45
Diuron	330-54-1	SH2060	284	99	34.86	21	7.39	11	3.87
Deisopropylatrazine	1007-28-9	SH2060	283	81	28.62	20	7.07	6	2.12
Triclopyr	55335-06-3	SH2060	284	37	13.03	19	6.69	11	3.87
(4-Chloro-2-methylphenoxy)-acetic acid (MCPA)	94-74-6	SH2060	282	38	13.48	13	4.61	7	2.48
Acetochlor	34256-82-1	SH2003/2033	279	44	15.77	8	2.87	7	2.51
3,4-Dichloroaniline	95-76-1	SH2003/2033	303	110	36.30	8	2.64	3	0.99
Dicamba	1918-00-9	SH2060	280	11	3.93	7	2.50	5	1.79
Propanil	709-98-8	SH2033	129	5	3.88	3	2.33	0	0.00
Prometon	1610-18-0	SH2003/2033	304	153	50.33	6	1.97	0	0.00
(2,4-Dichlorophenoxy) acetic acid, methyl ester (2,4-D methyl ester)	1928-38-7	SH2060	281	8	2.85	5	1.78	5	1.78
Metsulfuron methyl	74223-64-6	SH2060	267	3	1.12	3	1.12	0	0.00
Chlorimuron-ethyl	90982-32-4	SH2060	282	10	3.55	3	1.06	1	0.35
Imazethapyr	81335-77-5	SH2060	284	16	5.63	3	1.06	2	0.70
Molinate	2212-67-1	SH2033	129	7	5.43	1	0.78	1	0.78
Thiobencarb	28249-77-6	SH2033	129	6	4.65	1	0.78	1	0.78
Bentazon	25057-89-0	SH2060	284	22	7.75	2	0.70	1	0.35
Bromacil	314-40-9	SH2060	284	6	2.11	2	0.70	0	0.00
Metribuzin	21087-64-9	SH2003/2033	304	20	6.58	2	0.66	0	0.00
Flumetsulam	98967-40-9	SH2060	271	5	1.85	1	0.37	0	0.00



## Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Herbicides and herbicide degradates—Continued									
Picloram	1918-02-1	SH2060	274	1	0.36	1	0.36	1	0.36
Alachlor	15972-60-8	SH2003/2033	279	30	10.75	1	0.36	0	0.00
Imazaquin	81335-37-7	SH2060	282	15	5.32	1	0.35	1	0.35
Nicosulfuron	111991-09-4	SH2060	283	1	0.35	1	0.35	0	0.00
Dichlorprop	120-36-5	SH2060	284	9	3.17	1	0.35	0	0.00
Oryzalin	19044-88-3	SH2060	284	1	0.35	1	0.35	0	0.00
Terbutylazine	5915-41-3	SH2003/2033	304	51	16.78	0	0.00	0	0.00
Hexazinone	51235-04-2	SH2003/2033	238	39	16.39	0	0.00	0	0.00
Tebuthiuron	34014-18-1	SH2060/2033	304	29	9.54	0	0.00	0	0.00
Sulfometuron-methyl	74222-97-2	SH2060	282	17	6.03	0	0.00	0	0.00
Pendimethalin	40487-42-1	SH2003/2033	304	13	4.28	0	0.00	0	0.00
Dacthal	1861-32-1	SH2003/2033	304	11	3.62	0	0.00	0	0.00
4-Chloro-2-methylphenol	1570-64-5	SH2003/2033	304	10	3.29	0	0.00	0	0.00
Propyzamide	23950-58-5	SH2003/2033	304	8	2.63	0	0.00	0	0.00
Trifluralin	1582-09-8	SH2003/2033	304	8	2.63	0	0.00	0	0.00
Cyanazine	21725-46-2	SH2033	128	2	1.56	0	0.00	0	0.00
Eptam (EPTC)	759-94-4	SH2033	128	2	1.56	0	0.00	0	0.00
Siduron	1982-49-6	SH2060	284	4	1.41	0	0.00	0	0.00
2-Ethyl-6-methylamine	24549-06-2	SH2003/2033	303	4	1.32	0	0.00	0	0.00
Clopyralid	1702-17-6	SH2060	281	3	1.07	0	0.00	0	0.00
Fluometuron	2164-17-2	SH2060	284	3	1.06	0	0.00	0	0.00
Benfluralin	1861-40-1	SH2003/2033	304	3	0.99	0	0.00	0	0.00
Bromoxynil	1689-84-5	SH2060	282	2	0.71	0	0.00	0	0.00
Acifluorfen	50594-66-6	SH2060	282	1	0.35	0	0.00	0	0.00
Diphenamid	957-51-7	SH2060	282	1	0.35	0	0.00	0	0.00
Dinoseb	88-85-7	SH2060	284	1	0.35	0	0.00	0	0.00
Norflurazon	27314-13-2	SH2060	284	1	0.35	0	0.00	0	0.00

**Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Herbicides and herbicide degradates—Continued									
Terbacil	5902-51-2	SH2060	284	1	0.35	0	0.00	0	0.00
Prometryn	7287-19-6	SH2003/2033	304	1	0.33	0	0.00	0	0.00
4-(2,4-dichlorophenoxy)-butanoic acid (2,4-DB)	94-82-6	SH2060	284	0	0.00	0	0.00	0	0.00
3-(4-Chlorophenyl)-1-methyl urea	5352-88-5	SH2060	271	0	0.00	0	0.00	0	0.00
Bensulfuron-methyl	83055-99-6	SH2060	271	0	0.00	0	0.00	0	0.00
Chloramben, methyl ester	7286-84-2	SH2060	283	0	0.00	0	0.00	0	0.00
Cycloate	1134-23-2	SH2060	285	0	0.00	0	0.00	0	0.00
Dacthal monoacid	887-54-7	SH2060	284	0	0.00	0	0.00	0	0.00
Fenuron	101-42-8	SH2060	284	0	0.00	0	0.00	0	0.00
Linuron	330-55-2	SH2060	284	0	0.00	0	0.00	0	0.00
4-(2-methyl-4-chlorophenoxy) butyric acid (MCPB)	94-81-5	SH2060	284	0	0.00	0	0.00	0	0.00
Neburon	555-37-3	SH2060	284	0	0.00	0	0.00	0	0.00
Propham	122-42-9	SH2060	284	0	0.00	0	0.00	0	0.00
Oxyfluorfen	42874-03-3	SH2033	128	0	0.00	0	0.00	0	0.00
2,6-Diethylaniline	579-66-8	SH2003/2033	304	0	0.00	0	0.00	0	0.00
2-Chloro-2,6-diethylacetanilide	6967-29-9	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Insecticides and insecticide degradates									
Diazinon	333-41-5	SH2003/2033	304	72	23.68	3	0.99	0	0.00
Carbaryl	63-25-2	SH2060/2033	277	30	10.83	2	0.72	0	0.00
Imidacloprid	138261-41-3	SH2060	284	8	2.82	1	0.35	0	0.00
Fipronil	120068-37-3	SH2003/2033	304	90	29.61	0	0.00	0	0.00
Desulfnylfipronil	--	SH2003/2033	304	72	23.68	0	0.00	0	0.00
Fipronil sulfide	120067-83-6	SH2003/2033	304	50	16.45	0	0.00	0	0.00
Chlorpyrifos	2921-88-2	SH2003/2033	304	24	7.89	0	0.00	0	0.00
Fipronil sulfone	120068-36-2	SH2003/2033	304	24	7.89	0	0.00	0	0.00

## Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Insecticides and insecticide degradates—Continued									
1-Naphthol	90-15-3	SH2003/2033	304	19	6.25	0	0.00	0	0.00
Dichlorvos	62-73-7	SH2003/2033	304	10	3.29	0	0.00	0	0.00
Propoxur	114-26-1	SH2060	279	6	2.15	0	0.00	0	0.00
Malathion	121-75-5	SH2003/2033	304	6	1.97	0	0.00	0	0.00
Dimethoate	60-51-5	SH2003/2033	304	5	1.64	0	0.00	0	0.00
Propargite	2312-35-8	SH2033	128	2	1.56	0	0.00	0	0.00
Desulfynilfipronil amide	--	SH2003/2033	304	4	1.32	0	0.00	0	0.00
Carbofuran	1563-66-2	SH2060/2033	279	3	1.08	0	0.00	0	0.00
Dieldrin	60-57-1	SH2003/2033	304	2	0.66	0	0.00	0	0.00
Phosmet	732-11-6	SH2003/2033	280	1	0.36	0	0.00	0	0.00
Azinphos-methyl	86-50-0	SH2003/2033	304	1	0.33	0	0.00	0	0.00
3-Hydroxycarbofuran	16655-82-6	SH2060	279	0	0.00	0	0.00	0	0.00
Aldicarb	116-06-3	SH2060	282	0	0.00	0	0.00	0	0.00
Aldicarb sulfone	1646-88-4	SH2060	277	0	0.00	0	0.00	0	0.00
Aldicarb sulfoxide	1646-87-3	SH2060	277	0	0.00	0	0.00	0	0.00
Bendiocarb	22781-23-3	SH2060	277	0	0.00	0	0.00	0	0.00
Methiocarb	2032-65-7	SH2060	279	0	0.00	0	0.00	0	0.00
Methomyl	16752-77-5	SH2060	280	0	0.00	0	0.00	0	0.00
Oxamyl	23135-22-0	SH2060	276	0	0.00	0	0.00	0	0.00
<i>alpha</i> -Endosulfan	959-98-8	SH2033	128	0	0.00	0	0.00	0	0.00
Disulfoton	298-04-4	SH2033	128	0	0.00	0	0.00	0	0.00
Disulfoton sulfone	2497-06-5	SH2033	128	0	0.00	0	0.00	0	0.00
Endosulfan sulfate	1031-07-8	SH2033	128	0	0.00	0	0.00	0	0.00
Ethoprophos	13194-48-4	SH2033	128	0	0.00	0	0.00	0	0.00
<i>lambda</i> -Cyhalothrin	91465-08-6	SH2033	129	0	0.00	0	0.00	0	0.00
Tefluthrin	79538-32-2	SH2033	128	0	0.00	0	0.00	0	0.00
Azinphos-methyl-oxon	961-22-8	SH2003/2033	303	0	0.00	0	0.00	0	0.00

**Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Insecticides and insecticide degradates—Continued									
Chlorpyrifos, oxygen analog	5598-15-2	SH2003/2033	303	0	0.00	0	0.00	0	0.00
<i>cis</i> -Permethrin	61949-76-6	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Cyfluthrin	68359-37-5	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Cypermethrin	52315-07-8	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Diazinon, oxygen analog	962-58-3	SH2003/2033	303	0	0.00	0	0.00	0	0.00
Dicrotophos	141-66-2	SH2003/2033	300	0	0.00	0	0.00	0	0.00
Ethion	563-12-2	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Ethion monoxon	17356-42-2	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Fenamiphos	22224-92-6	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Fenamiphos sulfone	31972-44-8	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Fenamiphos sulfoxide	31972-43-7	SH2003/2033	298	0	0.00	0	0.00	0	0.00
Fonofos	944-22-9	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Isofenphos	25311-71-1	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Malaoxon	1634-78-2	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Methodathion	950-37-8	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Paraoxon-methyl	950-35-6	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Parathion-methyl	298-00-0	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Phorate	298-02-2	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Phorate oxon	2600-69-3	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Phosmet oxon	3735-33-9	SH2003/2033	262	0	0.00	0	0.00	0	0.00
Terbufos	13071-79-9	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Terbufos oxygen analogue sulfone	56070-15-6	SH2003/2033	304	0	0.00	0	0.00	0	0.00
Manufacturing additives									
Tri(2-butoxyethyl)phosphate	78-51-3	SH1433	298	71	23.83	71	23.83	67	22.48
Tris(dichloroisopropyl) phosphate	13674-87-8	SH1433	298	70	23.49	39	13.09	8	2.68
Tri(2-chloroethyl)phosphate	115-96-8	SH1433	298	8	2.68	8	2.68	8	2.68
5-Methyl-1 <i>H</i> -benzotriazole	136-85-6	SH1433	296	3	1.01	3	1.01	3	1.01

## Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Manufacturing additives—Continued									
Tributyl phosphate	126-73-8	SH1433	285	2	0.70	2	0.70	2	0.70
Triphenyl phosphate	115-86-6	SH1433	298	0	0.00	0	0.00	0	0.00
Organic synthesis compounds									
Anthraquinone	84-65-1	SH1433	298	14	4.70	10	3.36	3	1.01
Carbon disulfide	75-15-0	SH2020	300	7	2.33	2	0.67	1	0.33
Chloromethane	74-87-3	SH2020	300	7	2.33	2	0.67	1	0.33
Carbazole	86-74-8	SH1433	298	9	3.02	1	0.34	0	0.00
1,1-Dichloropropene	563-58-6	SH2020	300	0	0.00	0	0.00	0	0.00
1,2,3-Trichlorobenzene	87-61-6	SH2020	300	0	0.00	0	0.00	0	0.00
1,2,3-Trichloropropane	96-18-4	SH2020	300	0	0.00	0	0.00	0	0.00
3-Chloro-1-propene	107-05-1	SH2020	300	0	0.00	0	0.00	0	0.00
Acrylonitrile	107-13-1	SH2020	300	0	0.00	0	0.00	0	0.00
Ethyl methacrylate (ethyl 2-methyl-2-propanoate)	97-63-2	SH2020	300	0	0.00	0	0.00	0	0.00
Hexachlorobutadiene	87-68-3	SH2020	300	0	0.00	0	0.00	0	0.00
Iodomethane	74-88-4	SH2020	300	0	0.00	0	0.00	0	0.00
Methyl acrylate (methyl-2-propanoate)	96-33-3	SH2020	299	0	0.00	0	0.00	0	0.00
Methyl acrylonitrile (2-methyl-2-propene-nitrile)	126-98-7	SH2020	300	0	0.00	0	0.00	0	0.00
Methyl methacrylate (methyl 2-methyl-2-propanoate)	80-62-6	SH2020	300	0	0.00	0	0.00	0	0.00
<i>trans</i> -1,4-Dichloro-2-butene	110-57-6	SH2020	300	0	0.00	0	0.00	0	0.00
Vinyl bromide	593-60-2	SH2020	300	0	0.00	0	0.00	0	0.00
Vinyl chloride	75-01-4	SH2020	300	0	0.00	0	0.00	0	0.00
Pavement- and combustion-derived compounds									
Fluoranthene	206-44-0	SH1433	298	31	10.40	1	0.34	0	0.00
Pyrene	129-00-0	SH1433	298	28	9.40	0	0.00	0	0.00
Anthracene	120-12-7	SH1433	298	2	0.67	0	0.00	0	0.00

**Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Pavement- and combustion-derived compounds—Continued									
Benzo[ <i>a</i> ]pyrene	50–32–8	SH1433	298	1	0.34	0	0.00	0	0.00
Phenanthrene	85–01–8	SH1433	298	0	0.00	0	0.00	0	0.00
Personal-care and domestic-use products									
Hexahydrohexamethyl-cyclopentabenzopyran (HHCB)	1222–05–5	SH1433	298	95	31.88	88	29.53	29	9.73
Caffeine	58–08–2	SH2060	234	66	28.21	29	12.39	7	2.99
Nonylphenol, diethoxy- (total)	26027–38–2	SH1433	298	31	10.40	31	10.40	31	10.40
Acetyl hexamethyl tetrahydronaphthalene (AHTN)	21145–77–7	SH1433	298	76	25.50	28	9.40	1	0.34
Ocetylphenol, monoethoxy- (OPEO1)	2315–67–5	SH1433	298	21	7.05	21	7.05	18	6.04
Ocetylphenol, diethoxy- (OPEO2)	2315–61–9	SH1433	298	14	4.70	13	4.36	9	3.02
Triethyl citrate	77–93–0	SH1433	298	44	14.77	10	3.36	1	0.34
Triclosan	3380–34–5	SH1433	298	11	3.69	8	2.68	2	0.67
Cotinine	486–56–6	SH1433	298	16	5.37	6	2.01	3	1.01
Methyl salicylate	119–36–8	SH1433	270	2	0.74	2	0.74	1	0.37
Indole	120–72–9	SH1433	298	13	4.36	2	0.67	1	0.34
Menthol (5-methyl-2-[1-methylethyl]cyclohexanol)	89–78–1	SH1433	248	8	3.23	1	0.40	1	0.40
<i>d</i> -Limonene	5989–27–5	SH1433	298	5	1.68	1	0.34	0	0.00
Camphor	76–22–2	SH1433	282	32	11.35	0	0.00	0	0.00
4- <i>tert</i> -Octylphenol	140–66–9	SH1433	298	4	1.34	0	0.00	0	0.00
4-Cumylphenol	599–64–4	SH1433	298	1	0.34	0	0.00	0	0.00
Bromochloromethane	74–97–5	SH2020	300	0	0.00	0	0.00	0	0.00
3- <i>tert</i> -Butyl-4-hydroxy anisole (BHA)	25013–16–5	SH1433	276	0	0.00	0	0.00	0	0.00
4- <i>n</i> -Octylphenol	1806–26–4	SH1433	298	0	0.00	0	0.00	0	0.00
Acetophenone	98–86–2	SH1433	298	0	0.00	0	0.00	0	0.00
Isoborneol	124–76–5	SH1433	298	0	0.00	0	0.00	0	0.00
Isoquinoline	119–65–3	SH1433	297	0	0.00	0	0.00	0	0.00

## Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Plant- or animal-derived biochemicals									
Cholesterol	57-88-5	SH1433	295	56	18.98	56	18.98	56	18.98
3- <i>beta</i> -Coprostano	360-68-9	SH1433	298	27	9.06	27	9.06	27	9.06
<i>beta</i> -Stigmastanol	19466-47-8	SH1433	293	24	8.19	24	8.19	24	8.19
<i>beta</i> -Sitosterol	83-46-5	SH1433	295	22	7.46	22	7.46	22	7.46
3-Methyl-1( <i>H</i> )-indole (Skatole)	83-34-1	SH1433	298	11	3.69	1	0.34	0	0.00
Refrigerants and propellants									
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	76-13-1	SH2020	300	0	0.00	0	0.00	0	0.00
Dichlorodifluoromethane (CFC-12)	75-71-8	SH2020	300	0	0.00	0	0.00	0	0.00
Trichlorofluoromethane (CFC-11)	75-69-4	SH2020	300	0	0.00	0	0.00	0	0.00
Solvents									
<i>cis</i> -1,2-Dichloroethene	156-59-2	SH2020	300	46	15.33	15	5.00	7	2.33
<i>p</i> -Cresol	106-44-5	SH1433	298	45	15.10	14	4.70	4	1.34
Trichloroethene (TCE)	79-01-6	SH2020	300	47	15.67	13	4.33	0	0.00
Perchloroethene (PCE; tetrachloroethene)	127-18-4	SH2020	300	50	16.67	8	2.67	5	1.67
Chlorobenzene	108-90-7	SH2020	300	9	3.00	7	2.33	4	1.33
Acetone (2-propanone)	67-64-1	SH2020	287	4	1.39	4	1.39	4	1.39
Methylene chloride	75-09-2	SH2020	300	16	5.33	4	1.33	1	0.33
Tetrahydrofuran (1,4-epoxybutane)	109-99-9	SH2020	300	3	1.00	3	1.00	3	1.00
Diethyl ether (1,1'-oxybisethane)	60-29-7	SH2020	300	2	0.67	2	0.67	2	0.67
Methyl acetate	79-20-9	SH4024	298	1	0.34	1	0.34	0	0.00
Methyl ethyl ketone (MEK)	78-93-3	SH2020	299	1	0.33	1	0.33	1	0.33
<i>n</i> -Propylbenzene	103-65-1	SH2020	300	11	3.67	1	0.33	0	0.00
1,2-Dichlorobenzene ( <i>o</i> -dichlorobenzene)	95-50-1	SH2020	300	5	1.67	1	0.33	0	0.00
1,3-Dichlorobenzene ( <i>m</i> -dichlorobenzene)	541-73-1	SH2020	300	1	0.33	1	0.33	0	0.00
1,1,1-Trichloroethane	71-55-6	SH2020	300	1	0.33	0	0.00	0	0.00
Carbon tetrachloride	56-23-5	SH2020	300	1	0.33	0	0.00	0	0.00

**Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Solvents—Continued									
1,1,1,2-Tetrachloroethane	630–20–6	SH2020	300	0	0.00	0	0.00	0	0.00
1,1,2,2-Tetrachloroethane	79–34–5	SH2020	300	0	0.00	0	0.00	0	0.00
1,1,2-Trichloroethane	79–00–5	SH2020	300	0	0.00	0	0.00	0	0.00
1,1-Dichloroethane	75–34–3	SH2020	300	0	0.00	0	0.00	0	0.00
1,1-Dichloroethene	75–35–4	SH2020	300	0	0.00	0	0.00	0	0.00
1,2,4-Trichlorobenzene	120–82–1	SH2020	300	0	0.00	0	0.00	0	0.00
1,2-Dichloroethane (ethylene dichloride)	107–06–2	SH2020	300	0	0.00	0	0.00	0	0.00
2-Chlorotoluene	95–49–8	SH2020	300	0	0.00	0	0.00	0	0.00
2-Hexanone	591–78–6	SH2020	300	0	0.00	0	0.00	0	0.00
4-Chlorotoluene	106–43–4	SH2020	300	0	0.00	0	0.00	0	0.00
Bromobenzene	108–86–1	SH2020	300	0	0.00	0	0.00	0	0.00
Chloroethane	75–00–3	SH2020	300	0	0.00	0	0.00	0	0.00
Dibromomethane	74–95–3	SH2020	300	0	0.00	0	0.00	0	0.00
Hexachloroethane	67–72–1	SH2020	300	0	0.00	0	0.00	0	0.00
Methyl isobutyl ketone (MIBK) (4-methyl-2-pentanone)	108–10–1	SH2020	300	0	0.00	0	0.00	0	0.00
<i>trans</i> -1,2-Dichloroethene	156–60–5	SH2020	300	0	0.00	0	0.00	0	0.00
Additional herbicide and herbicide degradates									
Metolachlor ethane sulfonic acid	171118–09–5	LCPD	93	80	86.02	78	83.87	77	82.80
Metolachlor oxanilic acid	152019–73–3	LCPD	93	77	82.80	72	77.42	45	48.39
Alachlor ethane sulfonic acid	142363–53–9	LCPD	93	69	74.19	60	64.52	41	44.09
Acetochlor ethane sulfonic acid	187022–11–3	LCPD	93	60	64.52	54	58.06	44	47.31
Acetochlor oxanilic acid	184992–44–4	LCPD	93	54	58.06	48	51.61	35	37.63
Acetochlor/metolachlor ethane sulfonic acid 2nd amide	--	LCPD	60	36	60.00	16	26.67	2	3.33
Alachlor oxanilic acid	171262–17–2	LCPD	93	32	34.41	18	19.35	3	3.23
Acetochlor sulfamylacetic acid	--	LCPD	93	15	16.13	13	13.98	9	9.68
Dimethenamid ethane sulfonic acid	205939–58–8	LCPD	93	10	10.75	7	7.53	1	1.08



## Appendix 2. Summary of the frequency of detections in surface-water samples.—Continued

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstract Services Registry Number; USGS, U.S. Geological Survey; SH<sub>1</sub>, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples compound was analyzed	No assessment level		Assessment level of 0.05 microgram per liter		Assessment level of 0.1 microgram per liter	
				Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)	Number of detections in a sample	Detection frequency (percent)
Additional herbicide and herbicide degradates—Continued									
Alachlor sulfynilacetic acid	140939-16-8	LCPD	93	2	2.15	2	2.15	1	1.08
Dimethenamid oxanilic acid	--	LCPD	93	2	2.15	2	2.15	0	0.00
Alachlor ethane sulfonic acid 2nd amide	--	LCPD	60	4	6.67	1	1.67	0	0.00
Dimethenamid	87674-68-8	LCPD	59	2	3.39	0	0.00	0	0.00
Flufenacet ethane sulfonic acid	--	LCPD	93	1	1.08	0	0.00	0	0.00
Flufenacet	142459-58-3	LCPD	60	0	0.00	0	0.00	0	0.00
Flufenacet oxanilic acid	--	LCPD	93	0	0.00	0	0.00	0	0.00
Propachlor	1918-16-7	LCPD	43	0	0.00	0	0.00	0	0.00
Propachlor ethane sulfonic acid	--	LCPD	93	0	0.00	0	0.00	0	0.00
Propachlor oxanilic acid	--	LCPD	93	0	0.00	0	0.00	0	0.00

<sup>a</sup>This report contains Chemical Abstracts Service Registry Numbers (CASRN)<sup>®</sup>, which is a Registered Trademark of the American Chemical Society. The CASRN online database provides the latest registry number information: <http://www.cas.org/>. Chemical Abstracts Service recommends the verification of the CASRNs through CAS Client Services<sup>SM</sup>.

<sup>b</sup>Letter prefix added to CASRN because CASRN not available for *cis*- and *trans*-isomers.

## **Appendix 3. Summary of Frequency of Detections in Groundwater Samples**

### Appendix 3. Summary of frequency of detections in groundwater samples.

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Disinfection by-products									
Chloroform	67-66-3	SH2020	406	160	39.41	97	23.89	63	15.52
Bromodichloromethane	75-27-4	SH2020	448	32	7.14	19	4.24	10	2.23
Bromoform	75-25-2	SH2020	448	14	3.13	12	2.68	12	2.68
Dibromochloromethane	124-48-1	SH2020	448	13	2.90	12	2.68	11	2.46
Fumigant-related compounds									
1,2-Dibromo-3-chloropropane (DBCP)	96-12-8	SH2020	448	3	0.67	3	0.67	3	0.67
1,2-Dichloropropane	78-87-5	SH2020	448	6	1.34	2	0.45	0	0.00
1,2-Dibromoethane (EDB)	106-93-4	SH2020	448	1	0.22	1	0.22	0	0.00
1,4-Dichlorobenzene ( <i>p</i> -dichlorobenzene)	106-46-7	SH2020	448	3	0.67	0	0.00	0	0.00
1,3-Dichloropropane	142-28-9	SH2020	448	0	0.00	0	0.00	0	0.00
2,2-Dichloropropane	594-20-7	SH2020	448	0	0.00	0	0.00	0	0.00
Bromomethane (methyl bromide)	74-83-9	SH2020	448	0	0.00	0	0.00	0	0.00
<i>cis</i> -1,3-Dichloropropene	10061-01-5	SH2020	448	0	0.00	0	0.00	0	0.00
<i>trans</i> -1,3-Dichloropropene	10061-02-6	SH2020	448	0	0.00	0	0.00	0	0.00
Fungicides and fungicide degradates									
Metalaxyl	57837-19-1	SH2003/2033	445	7	1.57	1	0.22	1	0.22
3,5-Dichloroaniline	626-43-7	SH2033	221	4	1.81	0	0.00	0	0.00
Myclobutanil	88671-89-0	SH2003/2033	445	3	0.67	0	0.00	0	0.00
Propiconazole	60207-90-1	SH2060	440	2	0.45	0	0.00	0	0.00
<i>cis</i> -Propiconazole	c-60207-90-1 <sup>b</sup>	SH2033	221	1	0.45	0	0.00	0	0.00
<i>trans</i> -Propiconazole	t-60207-90-1 <sup>b</sup>	SH2033	221	1	0.45	0	0.00	0	0.00
Benomyl	17804-35-2	SH2060	440	0	0.00	0	0.00	0	0.00
Tebuconazole	107534-96-3	SH2033	209	0	0.00	0	0.00	0	0.00
Iprodione	36734-19-7	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Gasoline hydrocarbons, oxygenates, and oxygenate degradates									
Methyl <i>tert</i> -butyl ether (MTBE)	1634-04-4	SH2020	448	67	14.96	55	12.28	44	9.82
Benzene	71-43-2	SH2020	403	6	1.49	4	0.99	3	0.74

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Gasoline hydrocarbons, oxygenates, and oxygenate degradates—Continued									
<i>m</i> - & <i>p</i> -Xylene	<i>m</i> : 108-38-3; <i>p</i> : 106-42-3	SH2020	386	4	1.04	3	0.78	1	0.26
<i>tert</i> -Butyl alcohol	75-65-0	SH4024	447	3	0.67	3	0.67	3	0.67
<i>tert</i> -Amyl methyl ether (TAME)	994-05-8	SH2020	448	7	1.56	3	0.67	2	0.45
Ethylbenzene	100-41-4	SH2020	401	3	0.75	2	0.50	1	0.25
<i>o</i> -Xylene	95-47-6	SH2020	401	3	0.75	2	0.50	1	0.25
1,2,4-Trimethylbenzene	95-63-6	SH2020	402	5	1.24	2	0.50	1	0.25
Isopropylbenzene	98-82-8	SH2020	446	2	0.45	2	0.45	0	0.00
1-Ethyl-2-methylbenzene	611-14-3	SH2020	447	2	0.45	2	0.45	2	0.45
Naphthalene	91-20-3	SH2020	448	2	0.45	2	0.45	2	0.45
1-Methylnaphthalene	90-12-0	SH1433	441	3	0.68	1	0.23	1	0.23
2-Methylnaphthalene	91-57-6	SH1433	441	2	0.45	1	0.23	1	0.23
1,2,3,4-Tetramethylbenzene	488-23-3	SH2020	447	2	0.45	1	0.22	1	0.22
1,2,3,5-Tetramethylbenzene	527-53-7	SH2020	447	1	0.22	1	0.22	1	0.22
1,2,3-Trimethylbenzene	526-73-8	SH2020	447	1	0.22	1	0.22	1	0.22
1,3,5-Trimethylbenzene	108-67-8	SH2020	447	1	0.22	1	0.22	1	0.22
<i>n</i> -Butylbenzene	104-51-8	SH2020	447	1	0.22	1	0.22	0	0.00
<i>p</i> -Isopropyltoluene ( <i>p</i> -cymene)	99-87-6	SH2020	447	1	0.22	1	0.22	0	0.00
<i>sec</i> -Butylbenzene	135-98-8	SH2020	447	1	0.22	1	0.22	0	0.00
Diisopropyl ether (DIPE)	108-20-3	SH2020	448	1	0.22	1	0.22	1	0.22
2,6-Dimethylnaphthalene	581-42-0	SH1433	441	2	0.45	0	0.00	0	0.00
Styrene	100-42-5	SH2020	433	1	0.23	0	0.00	0	0.00
<i>tert</i> -Amyl alcohol (2-methyl-2-butanol)	75-85-4	SH4024	447	0	0.00	0	0.00	0	0.00
Ethyl <i>tert</i> -butyl ether (ETBE)	637-92-3	SH2020	448	0	0.00	0	0.00	0	0.00
<i>tert</i> -Butylbenzene	98-06-6	SH2020	448	0	0.00	0	0.00	0	0.00
Toluene	108-88-3	SH2020	295	0	0.00	0	0.00	0	0.00

## Appendix 3. Summary of frequency of detections in groundwater samples.—Continued

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Herbicides and herbicide degradates									
2-Hydroxyatrazine	2163-68-0	SH2060	436	45	10.32	17	3.90	11	2.52
Deethylatrazine	6190-65-4	SH2003/2033	443	144	32.51	15	3.39	6	1.35
Atrazine	1912-24-9	SH2003/2033	443	123	27.77	12	2.71	7	1.58
Tebuthiuron	34014-18-1	SH2060/2033	443	25	5.64	7	1.58	1	0.23
Diuron	330-54-1	SH2060	444	39	8.78	7	1.58	3	0.68
Bentazon	25057-89-0	SH2060	441	19	4.31	6	1.36	6	1.36
Hexazinone	51235-04-2	SH2003/2033	336	18	5.36	4	1.19	0	0.00
Deisopropylatrazine	1007-28-9	SH2060	444	34	7.66	4	0.90	1	0.23
Bromacil	314-40-9	SH2060	440	18	4.09	3	0.68	1	0.23
Simazine	122-34-9	SH2003/2033	445	62	13.93	3	0.67	3	0.67
Metolachlor	51218-45-2	SH2003/2033	415	17	4.10	2	0.48	0	0.00
Picloram	1918-02-1	SH2060	434	3	0.69	2	0.46	0	0.00
Alachlor	15972-60-8	SH2003/2033	430	4	0.93	1	0.23	1	0.23
Terbacil	5902-51-2	SH2060	440	1	0.23	1	0.23	0	0.00
3,4-Dichloroaniline	95-76-1	SH2003/2033	445	26	5.84	1	0.22	1	0.22
Prometon	1610-18-0	SH2003/2033	445	62	13.93	0	0.00	0	0.00
Eptam (EPTC)	759-94-4	SH2033	221	6	2.71	0	0.00	0	0.00
Diphenamid	957-51-7	SH2060	438	9	2.05	0	0.00	0	0.00
Imazaquin	81335-37-7	SH2060	442	7	1.58	0	0.00	0	0.00
Dinoseb	88-85-7	SH2060	440	6	1.36	0	0.00	0	0.00
Imazethapyr	81335-77-5	SH2060	440	4	0.91	0	0.00	0	0.00
Norflurazon	27314-13-2	SH2060	441	3	0.68	0	0.00	0	0.00
2-Ethyl-6-methylamine	24549-06-2	SH2003/2033	445	3	0.67	0	0.00	0	0.00
Metsulfuron methyl	74223-64-6	SH2060	425	2	0.47	0	0.00	0	0.00
Clopyralid	1702-17-6	SH2060	436	2	0.46	0	0.00	0	0.00
Bromoxynil	1689-84-5	SH2060	438	2	0.46	0	0.00	0	0.00
Sulfometuron-methyl	74222-97-2	SH2060	438	2	0.46	0	0.00	0	0.00

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Herbicides and herbicide degradates—Continued									
3-(4-Chlorophenyl)-1-methyl urea	5352-88-5	SH2060	440	2	0.45	0	0.00	0	0.00
Siduron	1982-49-6	SH2060	440	2	0.45	0	0.00	0	0.00
Thiobencarb	28249-77-6	SH2033	221	1	0.45	0	0.00	0	0.00
Fenuron	101-42-8	SH2060	444	2	0.45	0	0.00	0	0.00
2,6-Diethylaniline	579-66-8	SH2003/2033	445	2	0.45	0	0.00	0	0.00
Metribuzin	21087-64-9	SH2003/2033	445	2	0.45	0	0.00	0	0.00
Acetochlor	34256-82-1	SH2003/2033	430	1	0.23	0	0.00	0	0.00
(4-Chloro-2-methylphenoxy)-acetic acid (MCPA)	94-74-6	SH2060	432	1	0.23	0	0.00	0	0.00
Chloramben, methyl ester	7286-84-2	SH2060	436	1	0.23	0	0.00	0	0.00
2,4-Dichlorophenoxyacetic acid (2,4-D)	94-75-7	SH2060	440	1	0.23	0	0.00	0	0.00
Fluometuron	2164-17-2	SH2060	440	1	0.23	0	0.00	0	0.00
Terbutylazine	5915-41-3	SH2003/2033	444	1	0.23	0	0.00	0	0.00
4-Chloro-2-methylphenol	1570-64-5	SH2003/2033	445	1	0.22	0	0.00	0	0.00
Dacthal	1861-32-1	SH2003/2033	445	1	0.22	0	0.00	0	0.00
(2,4-Dichlorophenoxy) acetic acid, methyl ester (2,4-D methyl ester)	1928-38-7	SH2060	432	0	0.00	0	0.00	0	0.00
4-(2,4-dichlorophenoxy)-butanoic acid (2,4-DB)	94-82-6	SH2060	440	0	0.00	0	0.00	0	0.00
Acifluorfen	50594-66-6	SH2060	438	0	0.00	0	0.00	0	0.00
Bensulfuron-methyl	83055-99-6	SH2060	440	0	0.00	0	0.00	0	0.00
Chlorimuron-ethyl	90982-32-4	SH2060	438	0	0.00	0	0.00	0	0.00
Cycloate	1134-23-2	SH2060	440	0	0.00	0	0.00	0	0.00
Dacthal monoacid	887-54-7	SH2060	440	0	0.00	0	0.00	0	0.00
Dicamba	1918-00-9	SH2060	434	0	0.00	0	0.00	0	0.00
Dichlorprop	120-36-5	SH2060	440	0	0.00	0	0.00	0	0.00
Flumetsulam	98967-40-9	SH2060	440	0	0.00	0	0.00	0	0.00
Linuron	330-55-2	SH2060	440	0	0.00	0	0.00	0	0.00

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Herbicides and herbicide degradates—Continued									
4-(2-methyl-4-chlorophenoxy) butyric acid (MCPB)	94-81-5	SH2060	440	0	0.00	0	0.00	0	0.00
Neburon	555-37-3	SH2060	440	0	0.00	0	0.00	0	0.00
Nicosulfuron	111991-09-4	SH2060	440	0	0.00	0	0.00	0	0.00
Oryzalin	19044-88-3	SH2060	440	0	0.00	0	0.00	0	0.00
Propham	122-42-9	SH2060	439	0	0.00	0	0.00	0	0.00
Triclopyr	55335-06-3	SH2060	440	0	0.00	0	0.00	0	0.00
Cyanazine	21725-46-2	SH2033	221	0	0.00	0	0.00	0	0.00
Molinate	2212-67-1	SH2033	221	0	0.00	0	0.00	0	0.00
Oxyfluorfen	42874-03-3	SH2033	221	0	0.00	0	0.00	0	0.00
Propanil	709-98-8	SH2033	221	0	0.00	0	0.00	0	0.00
2-Chloro-2,6-diethylacetaniilide	6967-29-9	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Benfluralin	1861-40-1	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Pendimethalin	40487-42-1	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Prometryn	7287-19-6	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Propyzamide	23950-58-5	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Trifluralin	1582-09-8	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Insecticides and insecticide degradates									
Aldicarb sulfoxide	1646-87-3	SH2060	427	1	0.23	1	0.23	1	0.23
Aldicarb sulfone	1646-88-4	SH2060	432	2	0.46	1	0.23	1	0.23
Fipronil sulfide	120067-83-6	SH2003/2033	445	8	1.80	0	0.00	0	0.00
Carbofuran	1563-66-2	SH2060/2033	436	6	1.38	0	0.00	0	0.00
Dieldrin	60-57-1	SH2003/2033	445	6	1.35	0	0.00	0	0.00
Imidacloprid	138261-41-3	SH2060	440	5	1.14	0	0.00	0	0.00
Isofenphos	25311-71-1	SH2003/2033	445	3	0.67	0	0.00	0	0.00
Carbaryl	63-25-2	SH2060/2033	432	2	0.46	0	0.00	0	0.00
Propoxur	114-26-1	SH2060	437	2	0.46	0	0.00	0	0.00
Endosulfan sulfate	1031-07-8	SH2033	221	1	0.45	0	0.00	0	0.00

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Insecticides and insecticide degradates—Continued									
1-Naphthol	90–15–3	SH2003/2033	445	2	0.45	0	0.00	0	0.00
Desulfinylfipronil	--	SH2003/2033	445	2	0.45	0	0.00	0	0.00
Fipronil	120068–37–3	SH2003/2033	445	2	0.45	0	0.00	0	0.00
Bendiocarb	22781–23–3	SH2060	432	1	0.23	0	0.00	0	0.00
Chlorpyrifos, oxygen analog	5598–15–2	SH2003/2033	439	1	0.23	0	0.00	0	0.00
Chlorpyrifos	2921–88–2	SH2003/2033	445	1	0.22	0	0.00	0	0.00
Desulfinylfipronil amide	--	SH2003/2033	445	1	0.22	0	0.00	0	0.00
Fipronil sulfone	120068–36–2	SH2003/2033	445	1	0.22	0	0.00	0	0.00
3-Hydroxycarbofuran	16655–82–6	SH2060	436	0	0.00	0	0.00	0	0.00
Aldicarb	116–06–3	SH2060	440	0	0.00	0	0.00	0	0.00
Methiocarb	2032–65–7	SH2060	436	0	0.00	0	0.00	0	0.00
Methomyl	16752–77–5	SH2060	436	0	0.00	0	0.00	0	0.00
Oxamyl	23135–22–0	SH2060	432	0	0.00	0	0.00	0	0.00
<i>alpha</i> -Endosulfan	959–98–8	SH2033	221	0	0.00	0	0.00	0	0.00
Disulfoton	298–04–4	SH2033	221	0	0.00	0	0.00	0	0.00
Disulfoton sulfone	2497–06–5	SH2033	221	0	0.00	0	0.00	0	0.00
Ethoprophos	13194–48–4	SH2033	221	0	0.00	0	0.00	0	0.00
<i>lambda</i> -Cyhalothrin	91465–08–6	SH2033	221	0	0.00	0	0.00	0	0.00
Propargite	2312–35–8	SH2033	221	0	0.00	0	0.00	0	0.00
Tefluthrin	79538–32–2	SH2033	221	0	0.00	0	0.00	0	0.00
Azinphos-methyl	86–50–0	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Azinphos-methyl-oxon	961–22–8	SH2003/2033	444	0	0.00	0	0.00	0	0.00
<i>cis</i> -Permethrin	61949–76–6	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Cyfluthrin	68359–37–5	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Cypermethrin	52315–07–8	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Diazinon	333–41–5	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Diazinon, oxygen analog	962–58–3	SH2003/2033	433	0	0.00	0	0.00	0	0.00



**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Insecticides and insecticide degradates—Continued									
Dichlorvos	62-73-7	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Dicrotophos	141-66-2	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Dimethoate	60-51-5	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Ethion	563-12-2	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Ethion monoxon	17356-42-2	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Fenamiphos	22224-92-6	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Fenamiphos sulfone	31972-44-8	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Fenamiphos sulfoxide	31972-43-7	SH2003/2033	416	0	0.00	0	0.00	0	0.00
Fonofos	944-22-9	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Malaaxon	1634-78-2	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Malathion	121-75-5	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Methidathion	950-37-8	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Paraaxon-methyl	950-35-6	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Parathion-methyl	298-00-0	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Phorate	298-02-2	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Phorate oxon	2600-69-3	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Phosmet	732-11-6	SH2003/2033	423	0	0.00	0	0.00	0	0.00
Phosmet oxon	3735-33-9	SH2003/2033	377	0	0.00	0	0.00	0	0.00
Terbufos	13071-79-9	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Terbufos oxygen analogue sulfone	56070-15-6	SH2003/2033	445	0	0.00	0	0.00	0	0.00
Manufacturing additives									
Tributyl phosphate	126-73-8	SH1433	426	6	1.41	4	0.94	2	0.47
Triphenyl phosphate	115-86-6	SH1433	395	6	1.52	3	0.76	0	0.00
Tri(2-chloroethyl)phosphate	115-96-8	SH1433	411	4	0.97	0	0.00	0	0.00
Tris(dichloroisopropyl) phosphate	13674-87-8	SH1433	441	4	0.91	0	0.00	0	0.00
5-Methyl-1 <i>H</i> -benzotriazole	136-85-6	SH1433	439	0	0.00	0	0.00	0	0.00
Tri(2-butoxyethyl)phosphate	78-51-3	SH1433	426	0	0.00	0	0.00	0	0.00

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Organic synthesis compounds									
Carbon disulfide	75-15-0	SH2020	402	8	1.99	8	1.99	8	1.99
Vinyl chloride	75-01-4	SH2020	448	5	1.12	5	1.12	4	0.89
Chloromethane	74-87-3	SH2020	448	4	0.89	2	0.45	2	0.45
Anthraquinone	84-65-1	SH1433	441	1	0.23	1	0.23	1	0.23
Carbazole	86-74-8	SH1433	441	1	0.23	1	0.23	0	0.00
1,2,3-Trichloropropane	96-18-4	SH2020	448	1	0.22	1	0.22	1	0.22
Acrylonitrile	107-13-1	SH2020	448	1	0.22	1	0.22	1	0.22
1,1-Dichloropropene	563-58-6	SH2020	448	0	0.00	0	0.00	0	0.00
1,2,3-Trichlorobenzene	87-61-6	SH2020	448	0	0.00	0	0.00	0	0.00
3-Chloro-1-propene	107-05-1	SH2020	448	0	0.00	0	0.00	0	0.00
Ethyl methacrylate (ethyl 2-methyl-2-propanoate)	97-63-2	SH2020	448	0	0.00	0	0.00	0	0.00
Hexachlorobutadiene	87-68-3	SH2020	448	0	0.00	0	0.00	0	0.00
Iodomethane	74-88-4	SH2020	448	0	0.00	0	0.00	0	0.00
Methyl acrylate (methyl-2-propanoate)	96-33-3	SH2020	448	0	0.00	0	0.00	0	0.00
Methyl acrylonitrile (2-methyl-2-propene-nitrile)	126-98-7	SH2020	448	0	0.00	0	0.00	0	0.00
Methyl methacrylate (methyl 2-methyl-2-propanoate)	80-62-6	SH2020	448	0	0.00	0	0.00	0	0.00
<i>trans</i> -1,4-Dichloro-2-butene	110-57-6	SH2020	448	0	0.00	0	0.00	0	0.00
Vinyl bromide	593-60-2	SH2020	448	0	0.00	0	0.00	0	0.00
Pavement- and combustion-derived compounds									
Pyrene	129-00-0	SH1433	440	10	2.27	0	0.00	0	0.00
Fluoranthene	206-44-0	SH1433	441	9	2.04	0	0.00	0	0.00
Phenanthrene	85-01-8	SH1433	426	6	1.41	0	0.00	0	0.00
Anthracene	120-12-7	SH1433	441	2	0.45	0	0.00	0	0.00
Benzo[ <i>a</i> ]pyrene	50-32-8	SH1433	441	0	0.00	0	0.00	0	0.00

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Personal-care and domestic-use products—Continued									
4- <i>tert</i> -Octylphenol	140-66-9	SH1433	441	11	2.49	9	2.04	2	0.45
Menthol (5-methyl-2-[1-methylethyl]cyclohexanol)	89-78-1	SH1433	427	7	1.64	3	0.70	2	0.47
Octylphenol, diethoxy- (OPEO2)	2315-61-9	SH1433	441	4	0.91	3	0.68	2	0.45
Octylphenol, monoethoxy- (OPEO1)	2315-67-5	SH1433	441	3	0.68	3	0.68	3	0.68
Acetophenone	98-86-2	SH1433	407	1	0.25	1	0.25	1	0.25
Methyl salicylate	119-36-8	SH1433	441	5	1.13	1	0.23	1	0.23
4-Cumylphenol	599-64-4	SH1433	441	3	0.68	1	0.23	1	0.23
Indole	120-72-9	SH1433	441	2	0.45	1	0.23	0	0.00
Triclosan	3380-34-5	SH1433	441	1	0.23	1	0.23	0	0.00
Triethyl citrate	77-93-0	SH1433	441	1	0.23	1	0.23	1	0.23
Caffeine	58-08-2	SH2060	277	10	3.61	0	0.00	0	0.00
Hexahydrohexamethyl-cyclopentabenzopyran (HHCB)	1222-05-5	SH1433	411	9	2.19	0	0.00	0	0.00
Acetyl hexamethyl tetrahydronaphthalene (AHTN)	21145-77-7	SH1433	411	3	0.73	0	0.00	0	0.00
3- <i>tert</i> -Butyl-4-hydroxy anisole (BHA)	25013-16-5	SH1433	400	1	0.25	0	0.00	0	0.00
Camphor	76-22-2	SH1433	441	1	0.23	0	0.00	0	0.00
Bromochloromethane	74-97-5	SH2020	448	0	0.00	0	0.00	0	0.00
4- <i>n</i> -Octylphenol	1806-26-4	SH1433	441	0	0.00	0	0.00	0	0.00
Cotinine	486-56-6	SH1433	441	0	0.00	0	0.00	0	0.00
<i>d</i> -Limonene	5989-27-5	SH1433	441	0	0.00	0	0.00	0	0.00
Isoborneol	124-76-5	SH1433	441	0	0.00	0	0.00	0	0.00
Isoquinoline	119-65-3	SH1433	441	0	0.00	0	0.00	0	0.00
Nonylphenol, diethoxy- (total)	26027-38-2	SH1433	441	0	0.00	0	0.00	0	0.00
Plant- or animal-derived biochemicals									
<i>beta</i> -Sitosterol	83-46-5	SH1433	437	3	0.69	3	0.69	3	0.69
Cholesterol	57-88-5	SH1433	424	2	0.47	2	0.47	2	0.47

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Plant- or animal-derived biochemicals—Continued									
<i>beta</i> -Stigmastanol	19466–47–8	SH1433	439	2	0.46	2	0.46	2	0.46
3- <i>beta</i> -Coprostanol	360–68–9	SH1433	441	2	0.45	2	0.45	2	0.45
3-Methyl-1( <i>H</i> )-indole (Skatole)	83–34–1	SH1433	441	1	0.23	0	0.00	0	0.00
Refrigerants and propellants									
Trichlorofluoromethane (CFC-11)	75–69–4	SH2020	418	12	2.87	9	2.15	7	1.67
Dichlorodifluoromethane (CFC-12)	75–71–8	SH2020	448	10	2.23	9	2.01	4	0.89
1,1,2-Trichloro-1,2,2-trifluoroethane (CFC-113)	76–13–1	SH2020	448	9	2.01	6	1.34	5	1.12
Solvents									
Perchloroethene (PCE; tetrachloroethene)	127–18–4	SH2020	448	83	18.53	52	11.61	39	8.71
Trichloroethene (TCE)	79–01–6	SH2020	448	56	12.50	34	7.59	26	5.80
<i>cis</i> -1,2-Dichloroethene	156–59–2	SH2020	448	43	9.60	28	6.25	22	4.91
1,1,1-Trichloroethane	71–55–6	SH2020	448	37	8.26	20	4.46	13	2.90
1,1-Dichloroethane	75–34–3	SH2020	448	27	6.03	16	3.57	14	3.13
1,1-Dichloroethene	75–35–4	SH2020	448	21	4.69	15	3.35	10	2.23
1,2-Dichloroethane (ethylene dichloride)	107–06–2	SH2020	448	7	1.56	7	1.56	5	1.12
Carbon tetrachloride	56–23–5	SH2020	448	10	2.23	6	1.34	3	0.67
<i>trans</i> -1,2-Dichloroethene	156–60–5	SH2020	448	11	2.46	4	0.89	3	0.67
<i>p</i> -Cresol	106–44–5	SH1433	425	6	1.41	3	0.71	2	0.47
Chlorobenzene	108–90–7	SH2020	433	10	2.31	3	0.69	0	0.00
1,1,2-Trichloroethane	79–00–5	SH2020	447	3	0.67	2	0.45	0	0.00
Methyl ethyl ketone (MEK)	78–93–3	SH2020	447	2	0.45	2	0.45	2	0.45
Diethyl ether (1,1'-oxybisethane)	60–29–7	SH2020	448	2	0.45	2	0.45	1	0.22
Tetrahydrofuran (1,4-epoxybutane)	109–99–9	SH2020	448	2	0.45	2	0.45	2	0.45
Methylene chloride	75–09–2	SH2020	418	5	1.20	1	0.24	0	0.00
Acetone (2-propanone)	67–64–1	SH2020	447	1	0.22	1	0.22	1	0.22
Methyl isobutyl ketone (MIBK) (4-methyl-2-pentanone)	108–10–1	SH2020	447	1	0.22	1	0.22	1	0.22

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Solvents—Continued									
<i>n</i> -Propylbenzene	103-65-1	SH2020	447	1	0.22	1	0.22	1	0.22
Bromobenzene	108-86-1	SH2020	448	1	0.22	1	0.22	0	0.00
Dibromomethane	74-95-3	SH2020	448	1	0.22	1	0.22	0	0.00
1,2-Dichlorobenzene ( <i>o</i> -dichlorobenzene)	95-50-1	SH2020	448	1	0.22	0	0.00	0	0.00
Methyl acetate	79-20-9	SH4024	447	0	0.00	0	0.00	0	0.00
1,1,1,2-Tetrachloroethane	630-20-6	SH2020	448	0	0.00	0	0.00	0	0.00
1,1,2,2-Tetrachloroethane	79-34-5	SH2020	448	0	0.00	0	0.00	0	0.00
1,2,4-Trichlorobenzene	120-82-1	SH2020	448	0	0.00	0	0.00	0	0.00
1,3-Dichlorobenzene ( <i>m</i> -dichlorobenzene)	541-73-1	SH2020	448	0	0.00	0	0.00	0	0.00
2-Chlorotoluene	95-49-8	SH2020	448	0	0.00	0	0.00	0	0.00
2-Hexanone	591-78-6	SH2020	448	0	0.00	0	0.00	0	0.00
4-Chlorotoluene	106-43-4	SH2020	448	0	0.00	0	0.00	0	0.00
Chloroethane	75-00-3	SH2020	448	0	0.00	0	0.00	0	0.00
Hexachloroethane	67-72-1	SH2020	448	0	0.00	0	0.00	0	0.00
Additional herbicide and herbicide degradates									
Metolachlor ethane sulfonic acid	171118-09-5	LCPD	118	27	22.88	23	19.49	18	15.25
Alachlor ethane sulfonic acid	142363-53-9	LCPD	118	28	23.73	20	16.95	13	11.02
Metolachlor oxanilic acid	152019-73-3	LCPD	118	15	12.71	12	10.17	9	7.63
Alachlor ethane sulfonic acid 2nd amide	--	LCPD	88	6	6.82	3	3.41	0	0.00
Alachlor oxanilic acid	171262-17-2	LCPD	118	5	4.24	3	2.54	2	1.69
Acetochlor ethane sulfonic acid	187022-11-3	LCPD	118	2	1.69	2	1.69	1	0.85
Acetochlor oxanilic acid	184992-44-4	LCPD	118	2	1.69	2	1.69	2	1.69
Dimethenamid ethane sulfonic acid	205939-58-8	LCPD	118	1	0.85	1	0.85	0	0.00
Acetochlor/metolachlor ethane sulfonic acid 2nd amide	--	LCPD	88	1	1.14	0	0.00	0	0.00
Dimethenamid oxanilic acid	--	LCPD	118	1	0.85	0	0.00	0	0.00

**Appendix 3. Summary of frequency of detections in groundwater samples.—Continued**

[Compounds are listed in order of decreasing detection frequency for an assessment level of 0.05 microgram per liter. CASRN, Chemical Abstracts Service Registry Number; USGS, U.S. Geological Survey; SH, laboratory schedule]

Compound name	CASRN <sup>a</sup>	USGS schedule	Number of samples of compound was analyzed	No assessment level		Assessment level of 0.05 micrograms per liter		Assessment level of 0.1 micrograms per liter	
				Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency	Number of detections in a sample	Detection frequency
Additional herbicide and herbicide degradates—Continued									
Acetochlor sulfynilacetic acid	--	LCPD	118	0	0.00	0	0.00	0	0.00
Alachlor sulfynilacetic acid	140939-16-8	LCPD	118	0	0.00	0	0.00	0	0.00
Dimethenamid	87674-68-8	LCPD	88	0	0.00	0	0.00	0	0.00
Flufenacet	142459-58-3	LCPD	88	0	0.00	0	0.00	0	0.00
Flufenacet ethane sulfonic acid	--	LCPD	118	0	0.00	0	0.00	0	0.00
Flufenacet oxanilic acid	--	LCPD	118	0	0.00	0	0.00	0	0.00
Propachlor	1918-16-7	LCPD	60	0	0.00	0	0.00	0	0.00
Propachlor ethane sulfonic acid	--	LCPD	118	0	0.00	0	0.00	0	0.00
Propachlor oxanilic acid	--	LCPD	118	0	0.00	0	0.00	0	0.00

<sup>a</sup>This report contains Chemical Abstracts Service Registry Numbers (CASRN)<sup>®</sup>, which is a Registered Trademark of the American Chemical Society. The CASRN online database provides the latest registry number information: <http://www.cas.org/>. Chemical Abstracts Service recommends the verification of the CASRNs through CAS Client Services<sup>SM</sup>.

<sup>b</sup>Letter prefix added to CASRN because CASRN not available for *cis*- and *trans*-isomers.

## Appendix 4. Qualified Concentrations of Compounds Monitored in Surface Water During 2002–10 by Primary Use Group And Human-Health Benchmarks (Where Applicable)

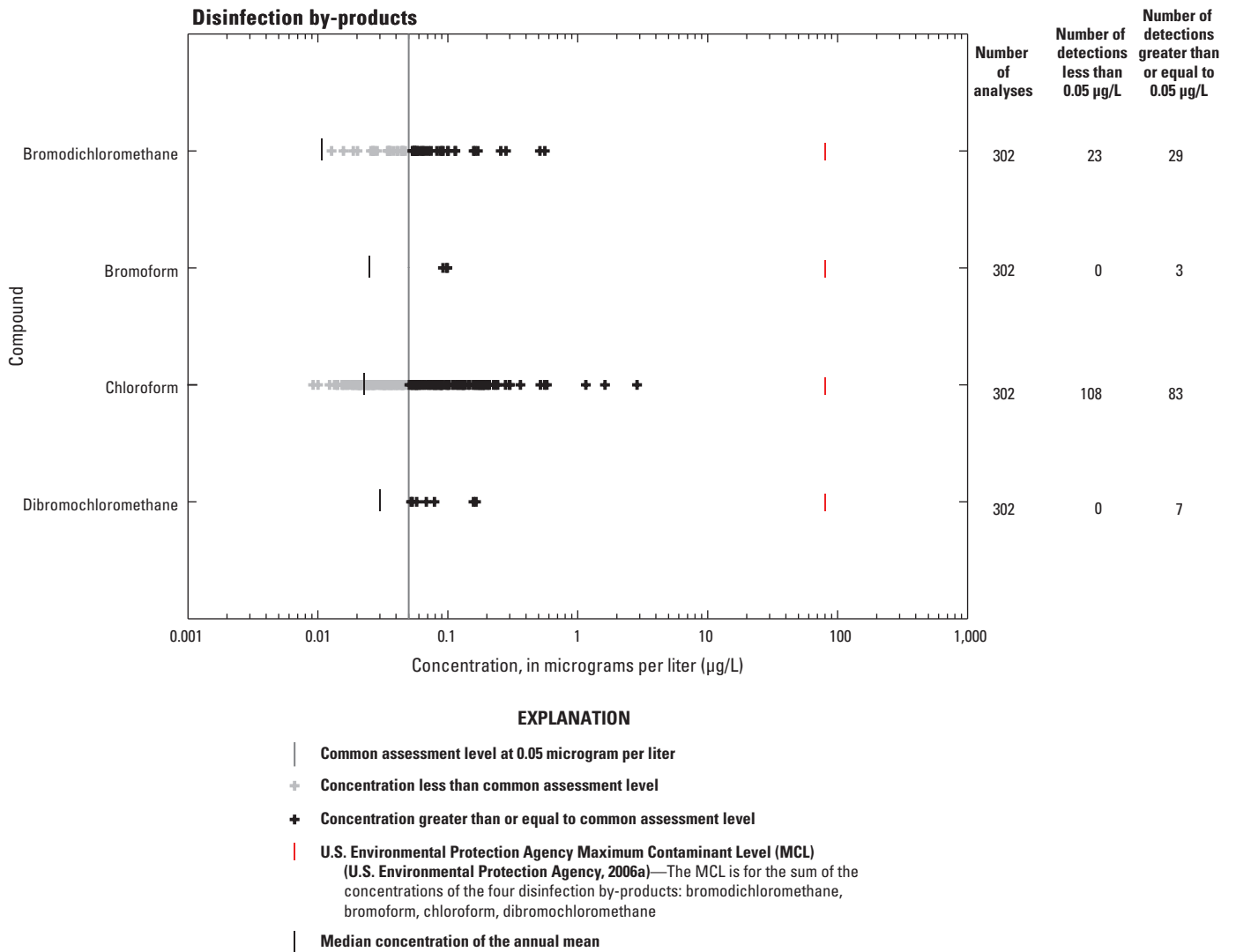
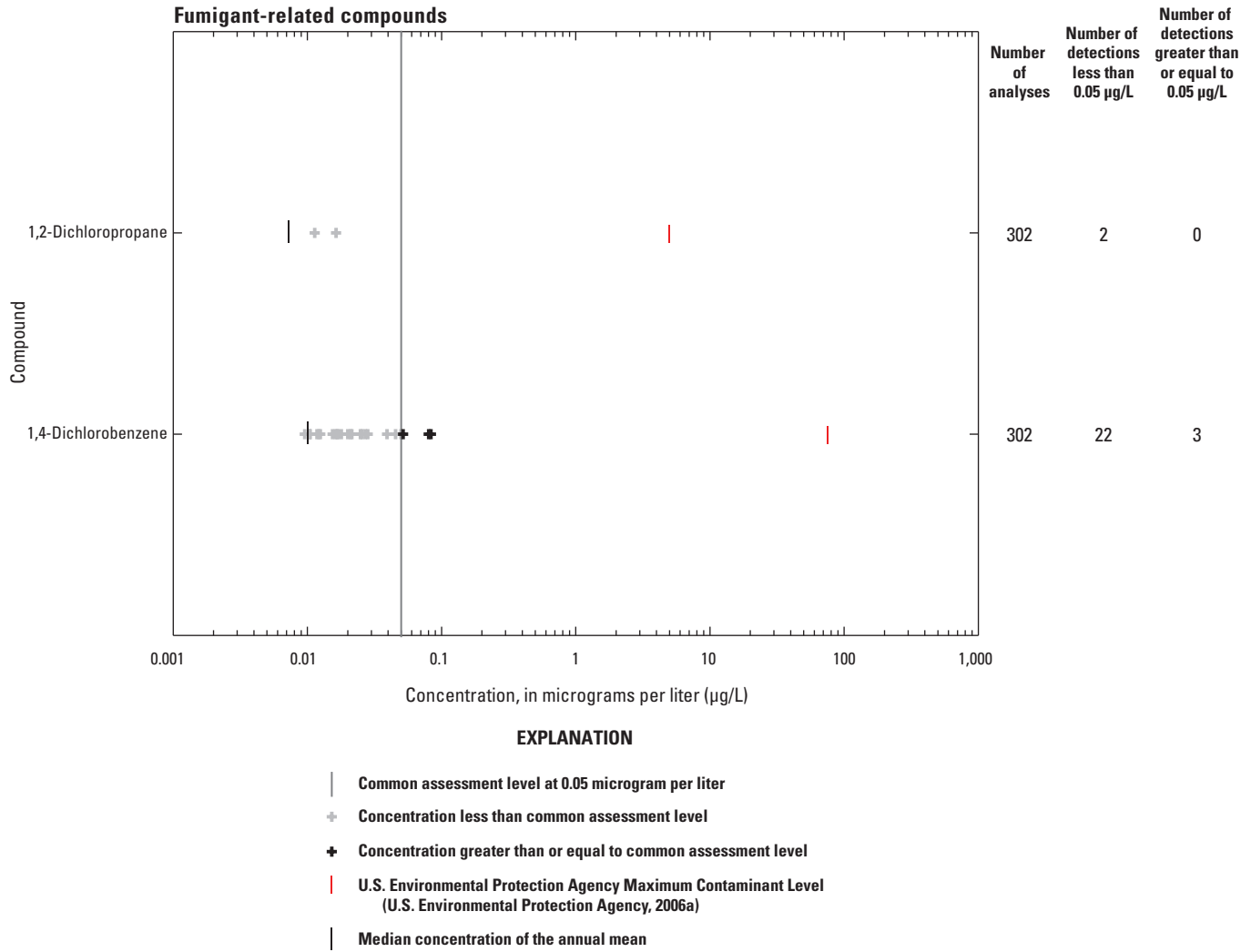
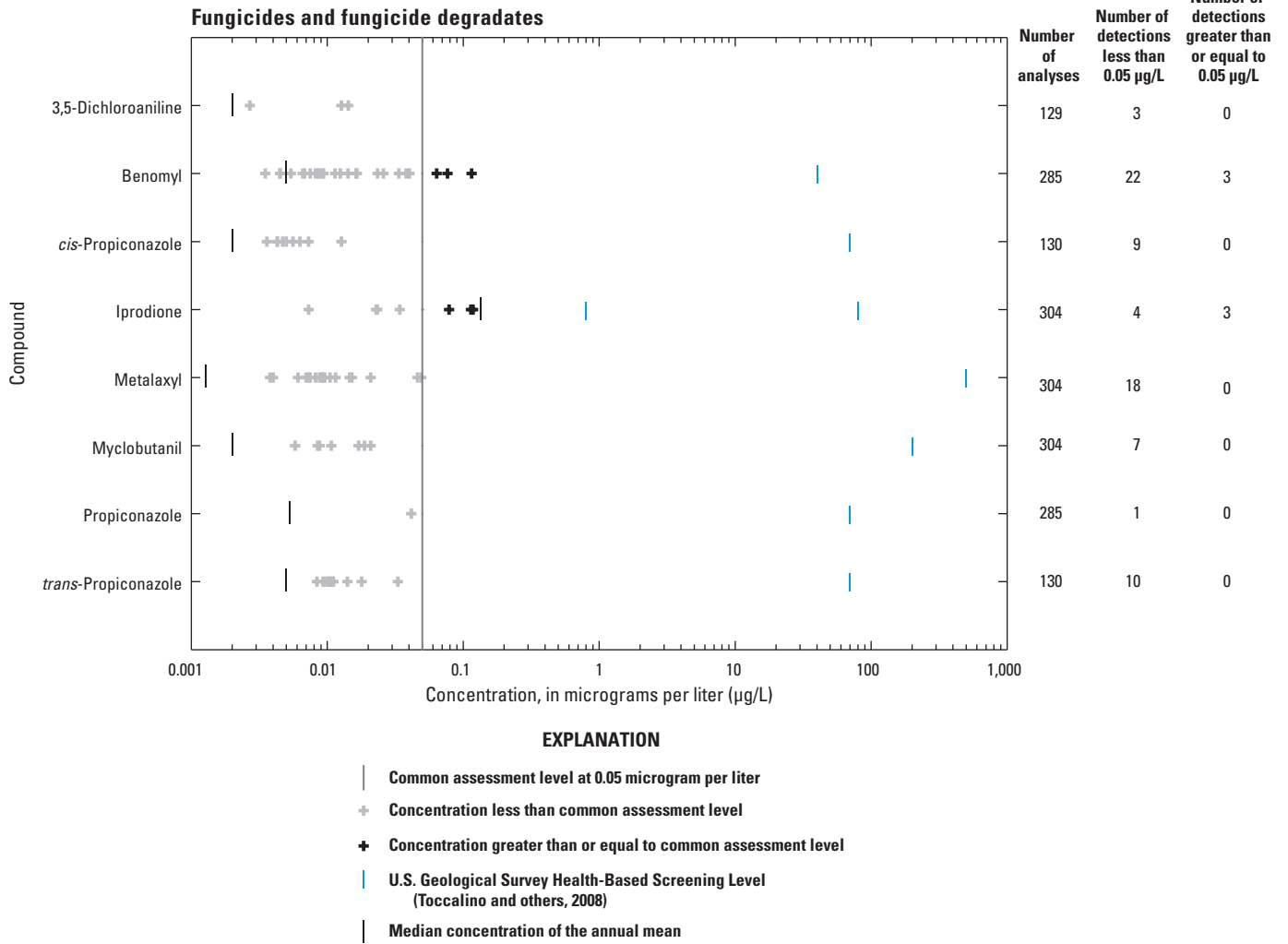


Figure 4–1. Qualified concentrations of disinfection by-products in surface water, 2002–10.



**Figure 4–2.** Qualified concentrations of fumigant-related compounds in surface water, 2002–10.





**Figure 4–3.** Qualified concentrations of fungicides and fungicide degradates compounds in surface water, 2002–10.

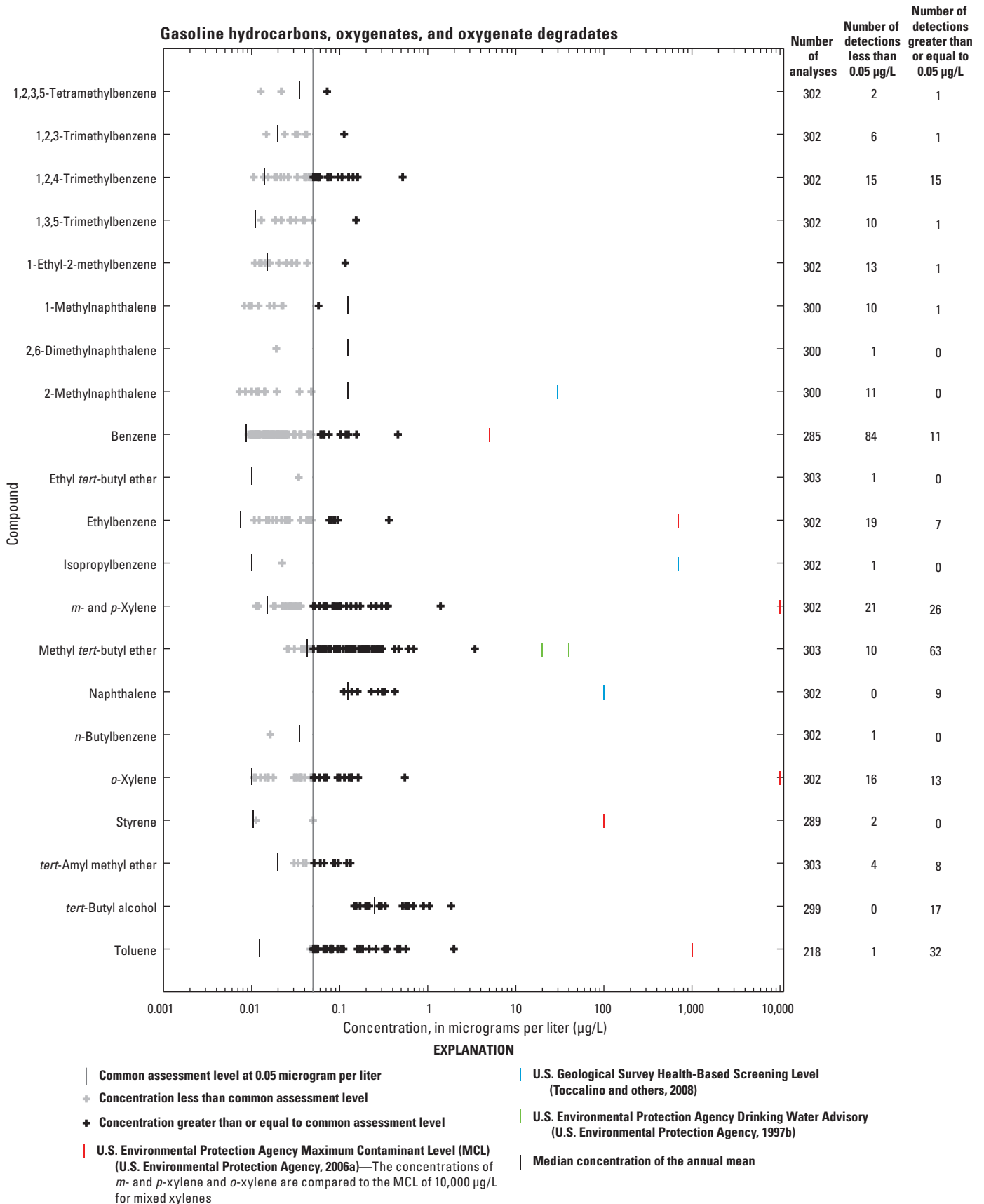


Figure 4–4. Qualified concentrations of gasoline hydrocarbons, oxygenates, and oxygenate degradates in surface water, 2002–10.

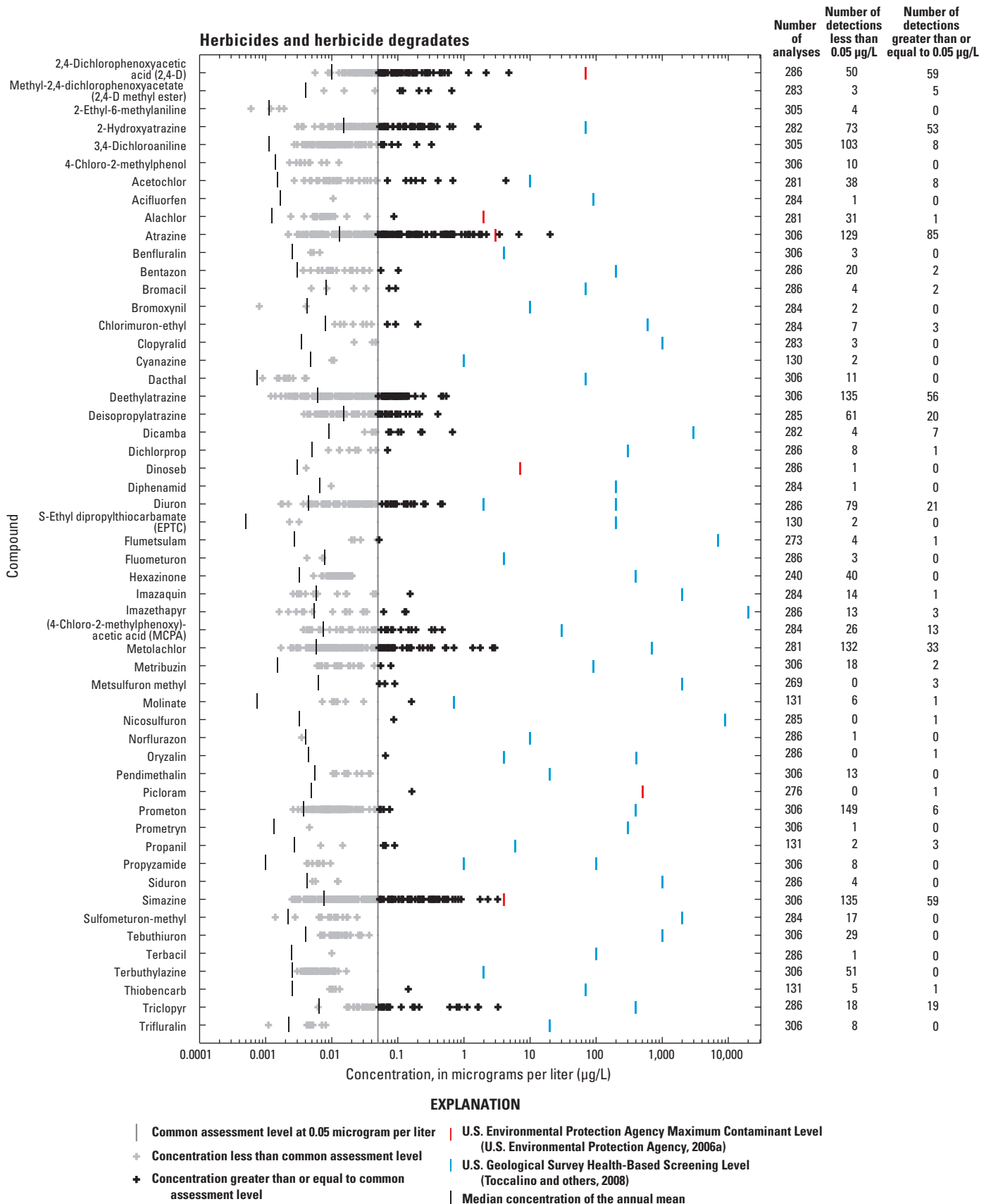


Figure 4-5. Qualified concentrations of herbicides and herbicide degradates in surface water, 2002–10.

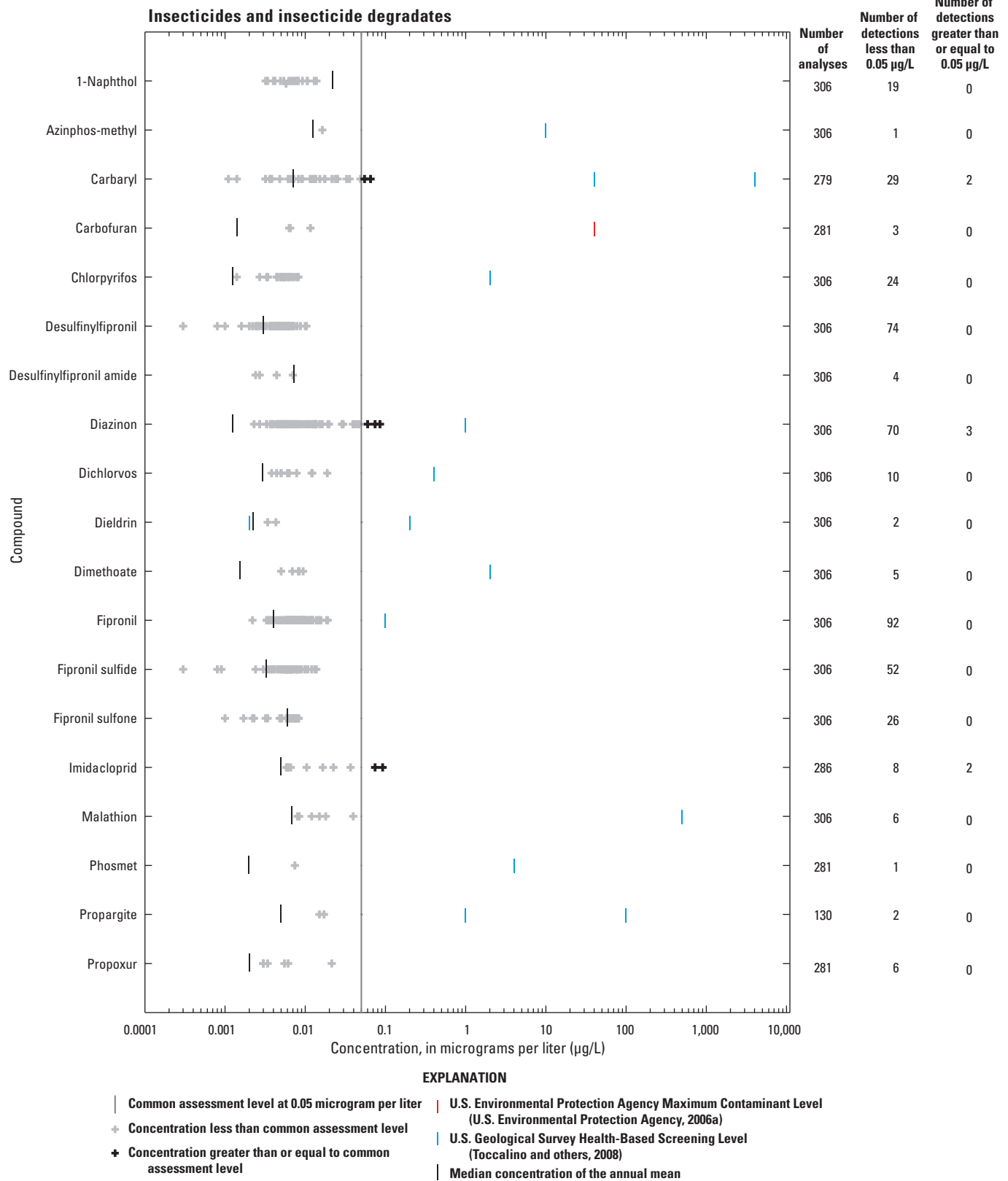


Figure 4–6. Qualified concentrations of insecticides and insecticide degradates in surface water, 2002–10.

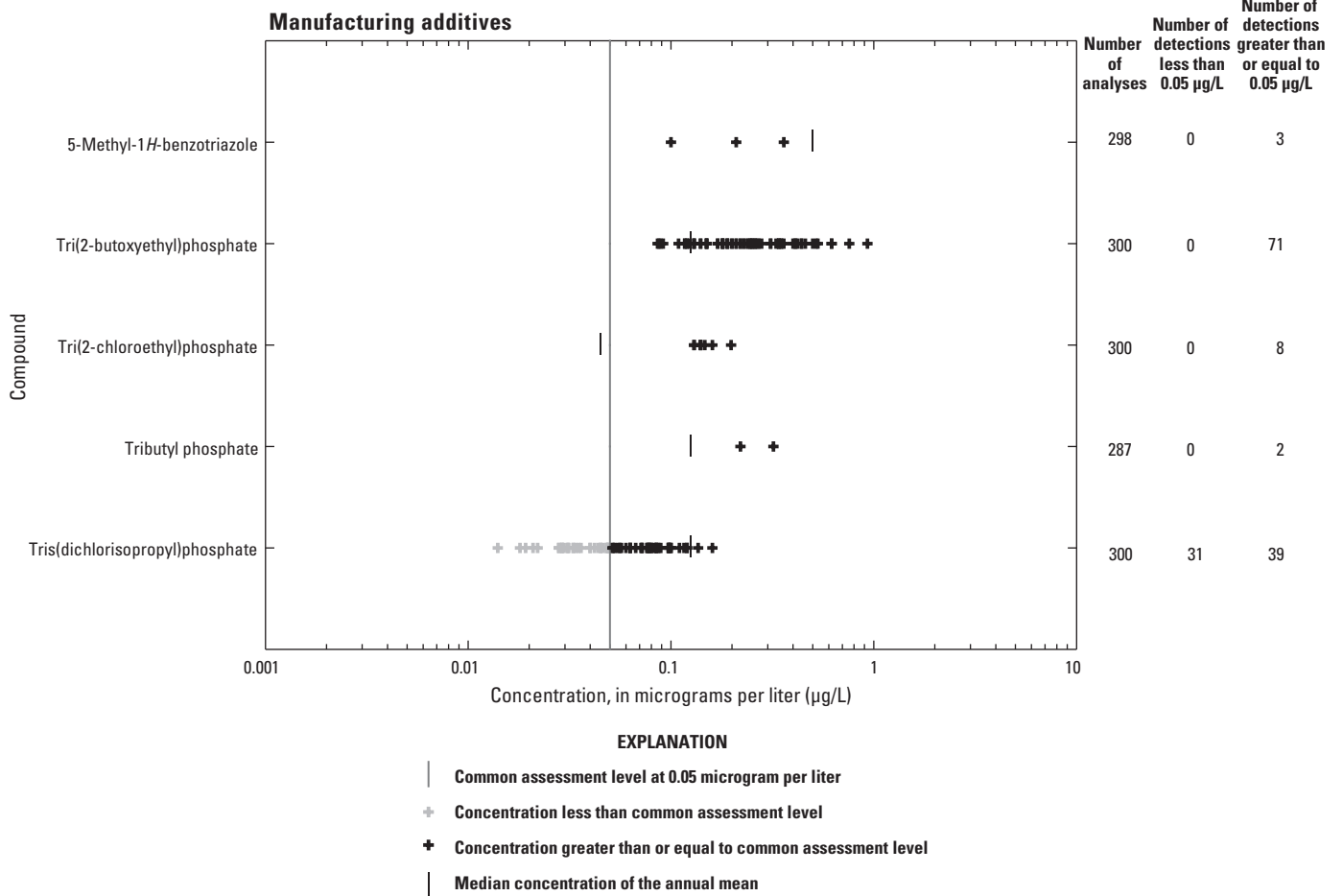


Figure 4-7. Qualified concentrations of manufacturing additives in surface water, 2002-10.

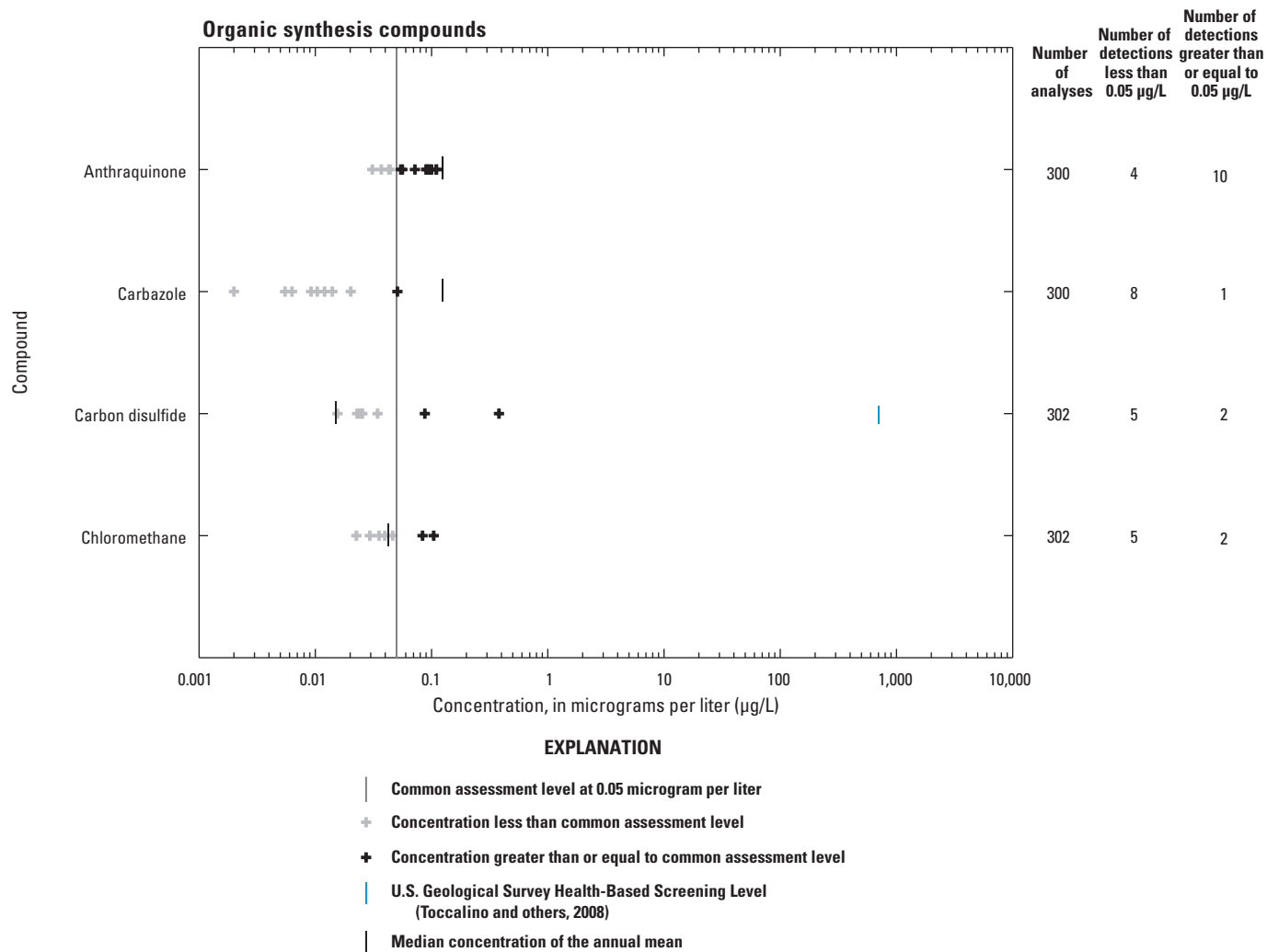
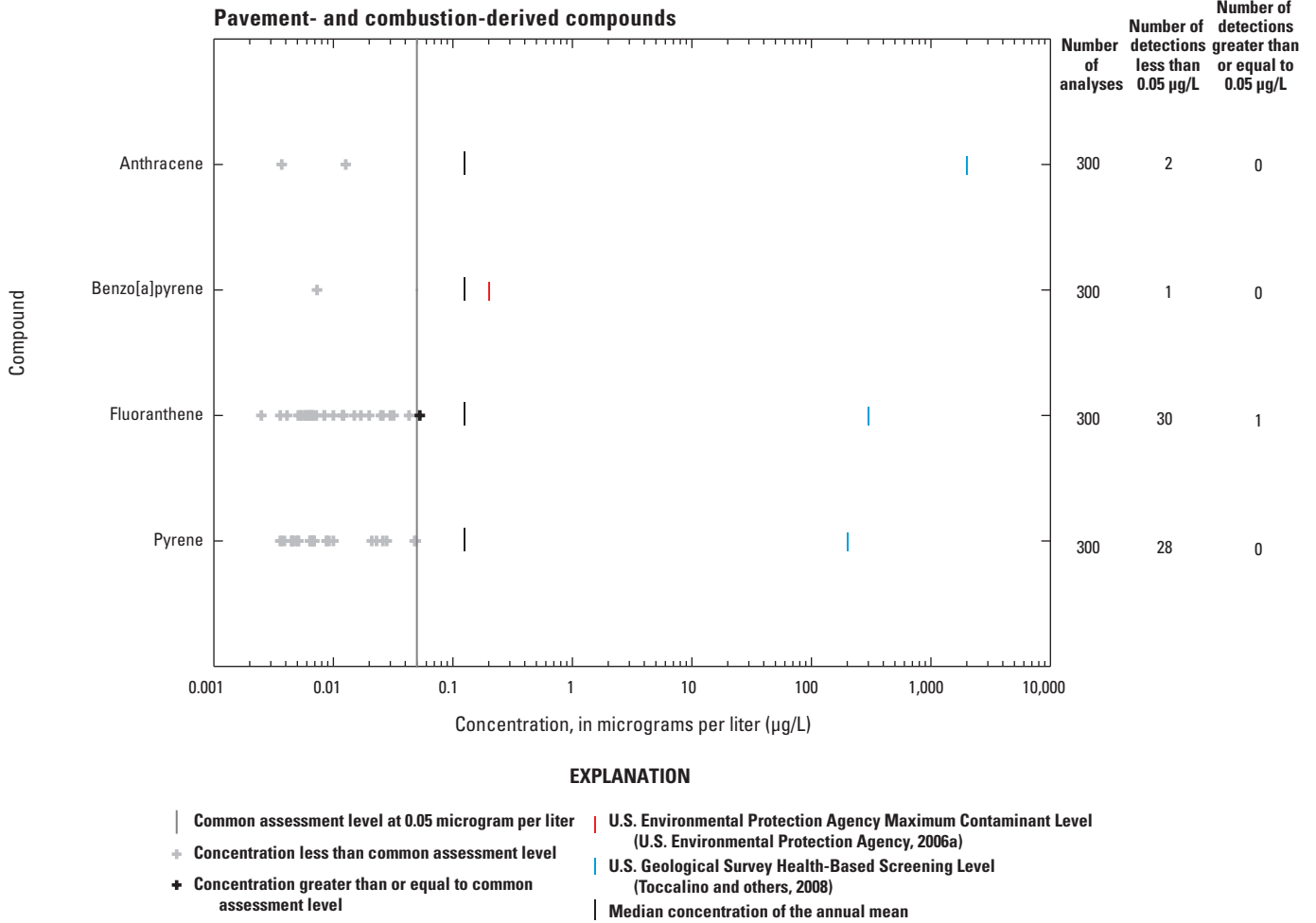


Figure 4–8. Qualified concentrations of organic synthesis compounds in surface water, 2002–10.



**Figure 4-9.** Qualified concentrations of pavement- and combustion-derived compounds in surface water, 2002–10.

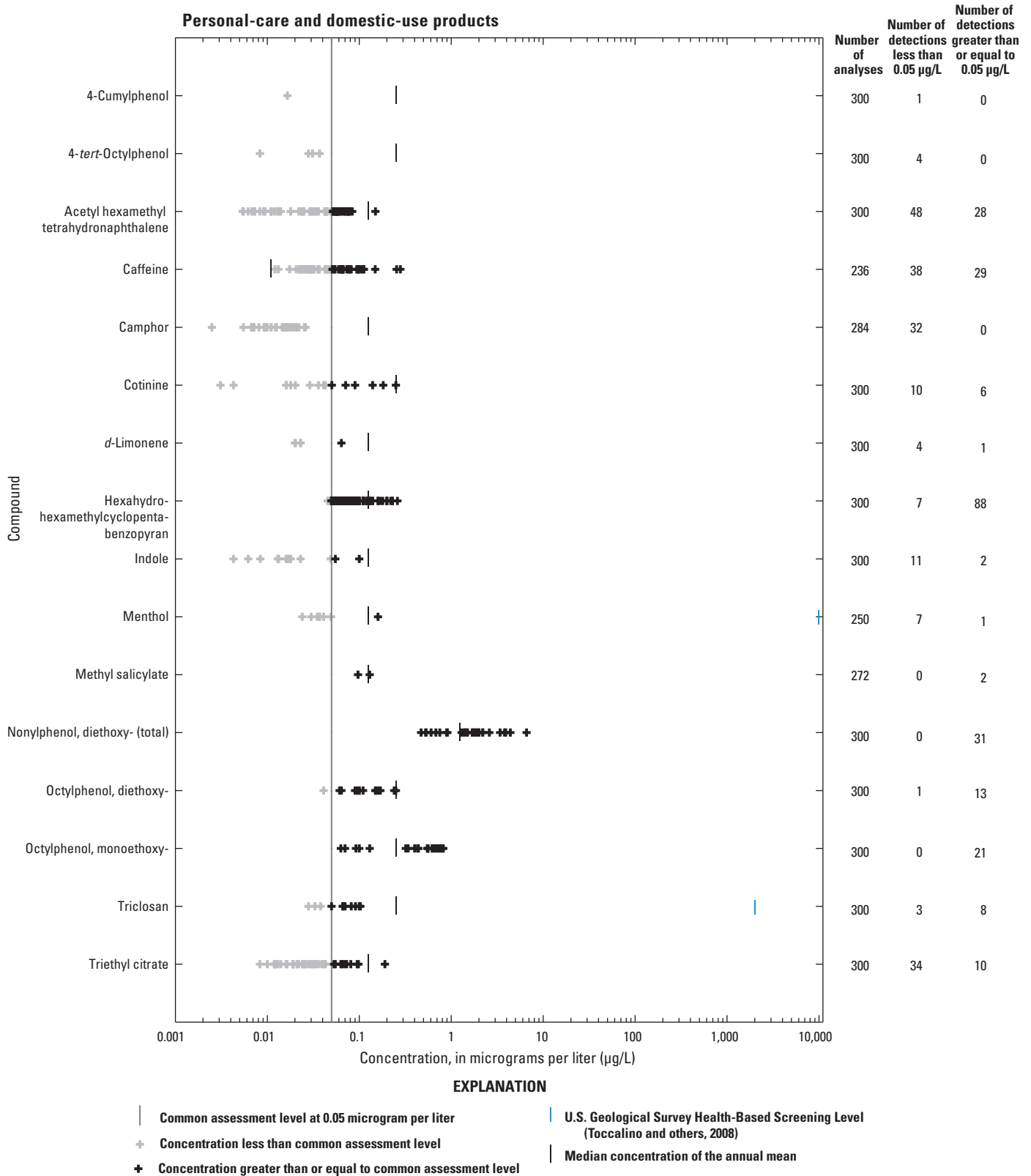
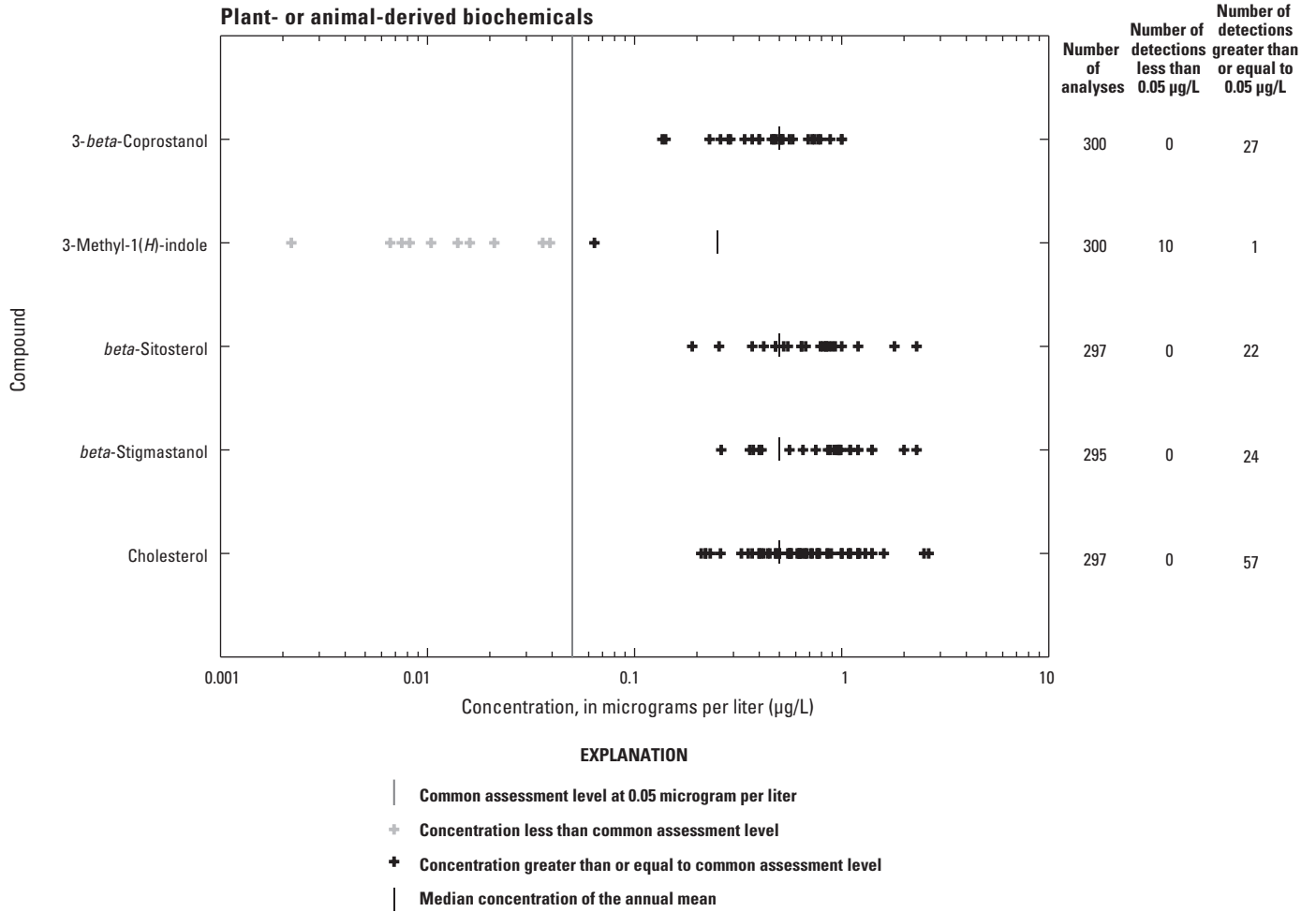


Figure 4–10. Qualified concentrations of personal-care and domestic-use products in surface water, 2002–10.





**Figure 4–11.** Qualified concentrations of plant- or animal-derived biochemicals in surface water, 2002–10.

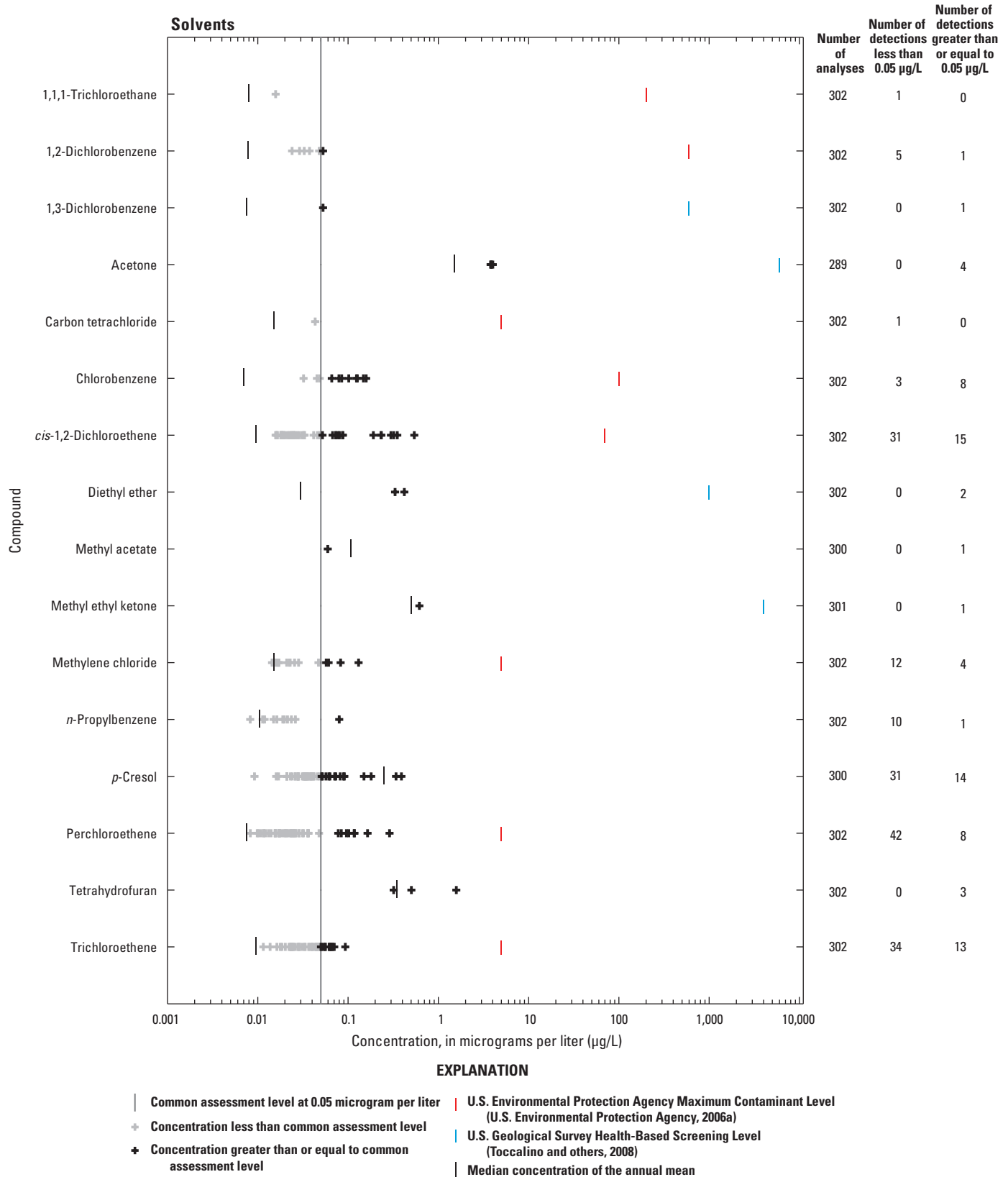


Figure 4–12. Qualified concentrations of of solvents in surface water, 2002–10.

## Appendix 5. Qualified Concentrations of Compounds Monitored in Groundwater During 2002–09 by Primary Use Group and Human-Health Benchmarks (Where Applicable)

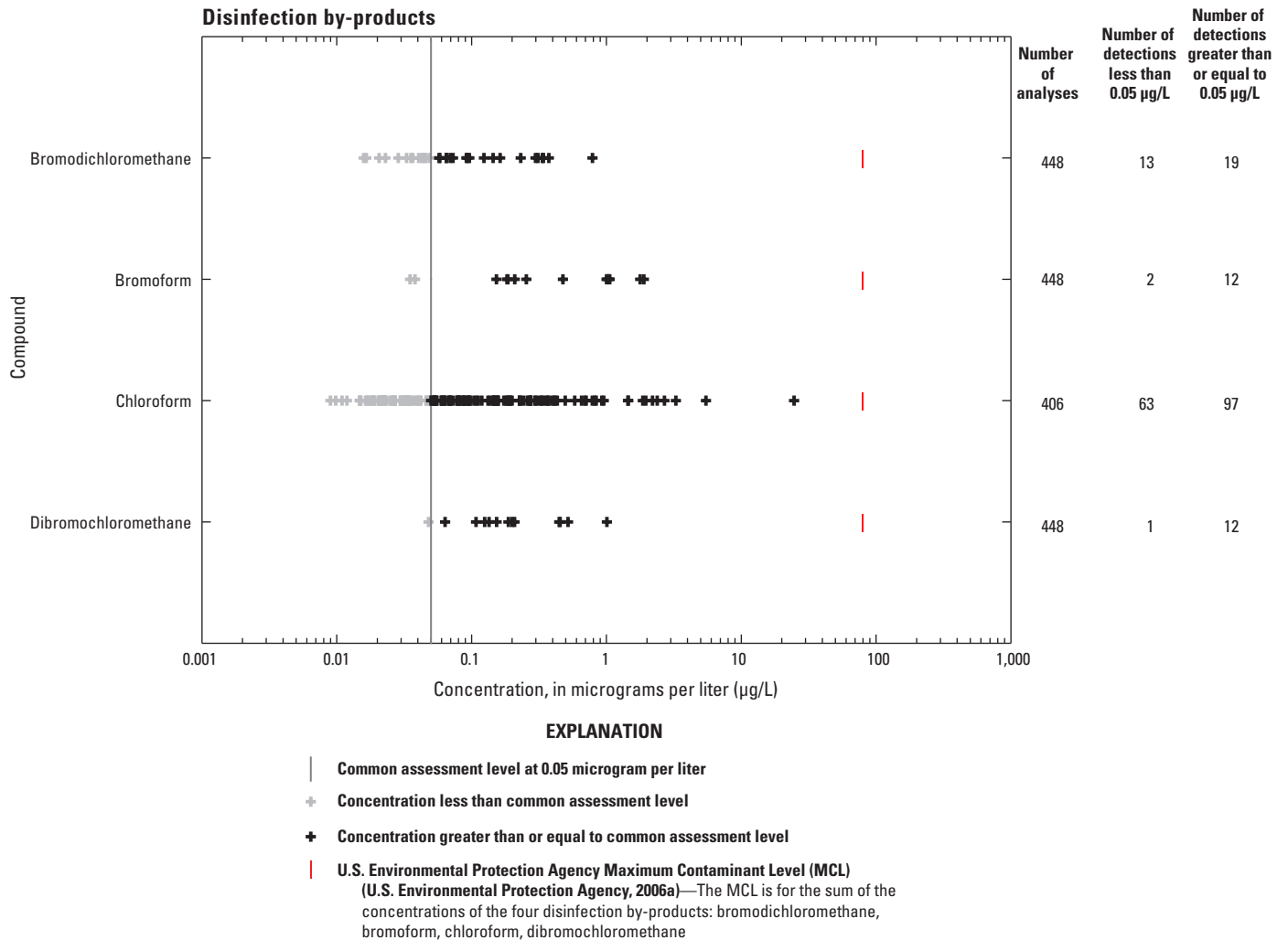
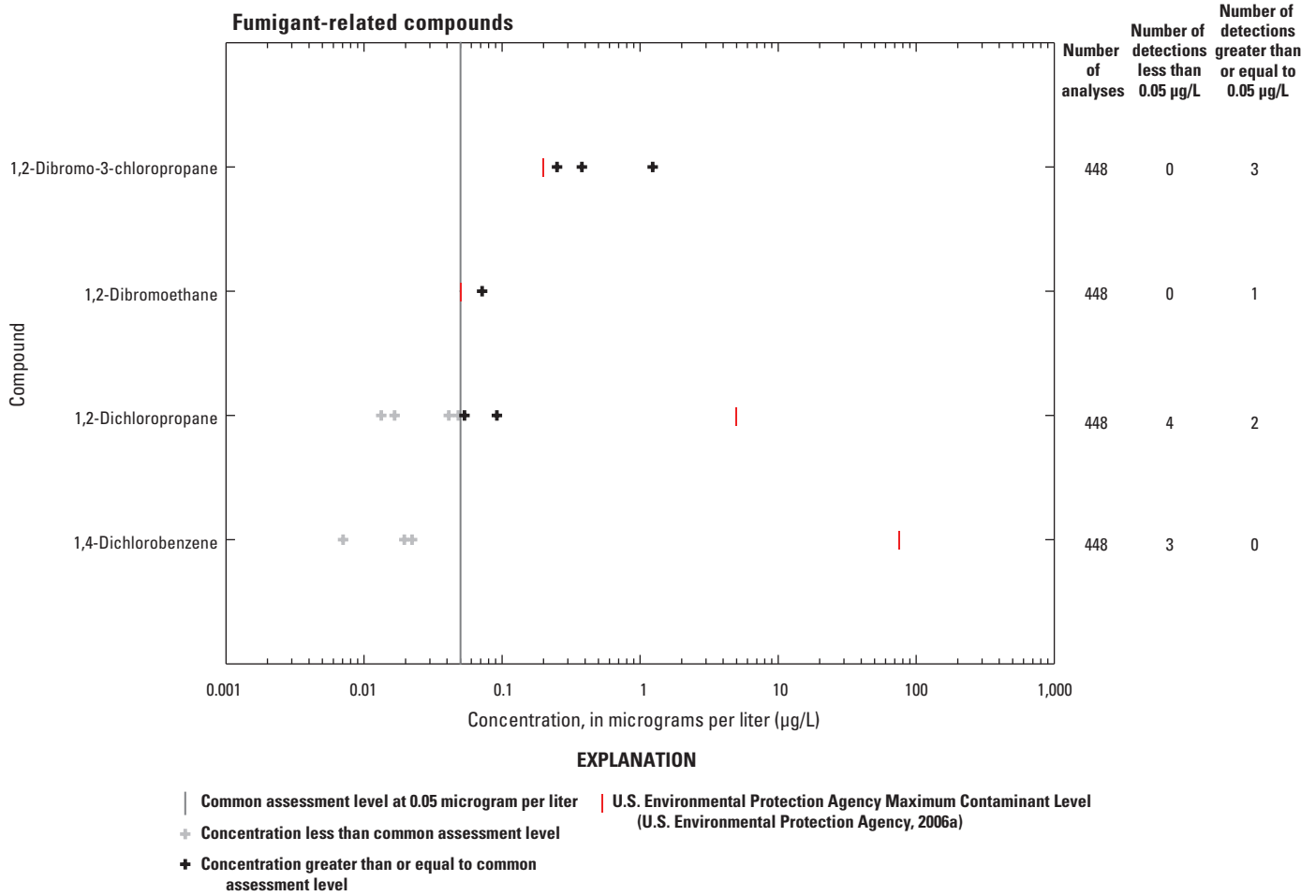
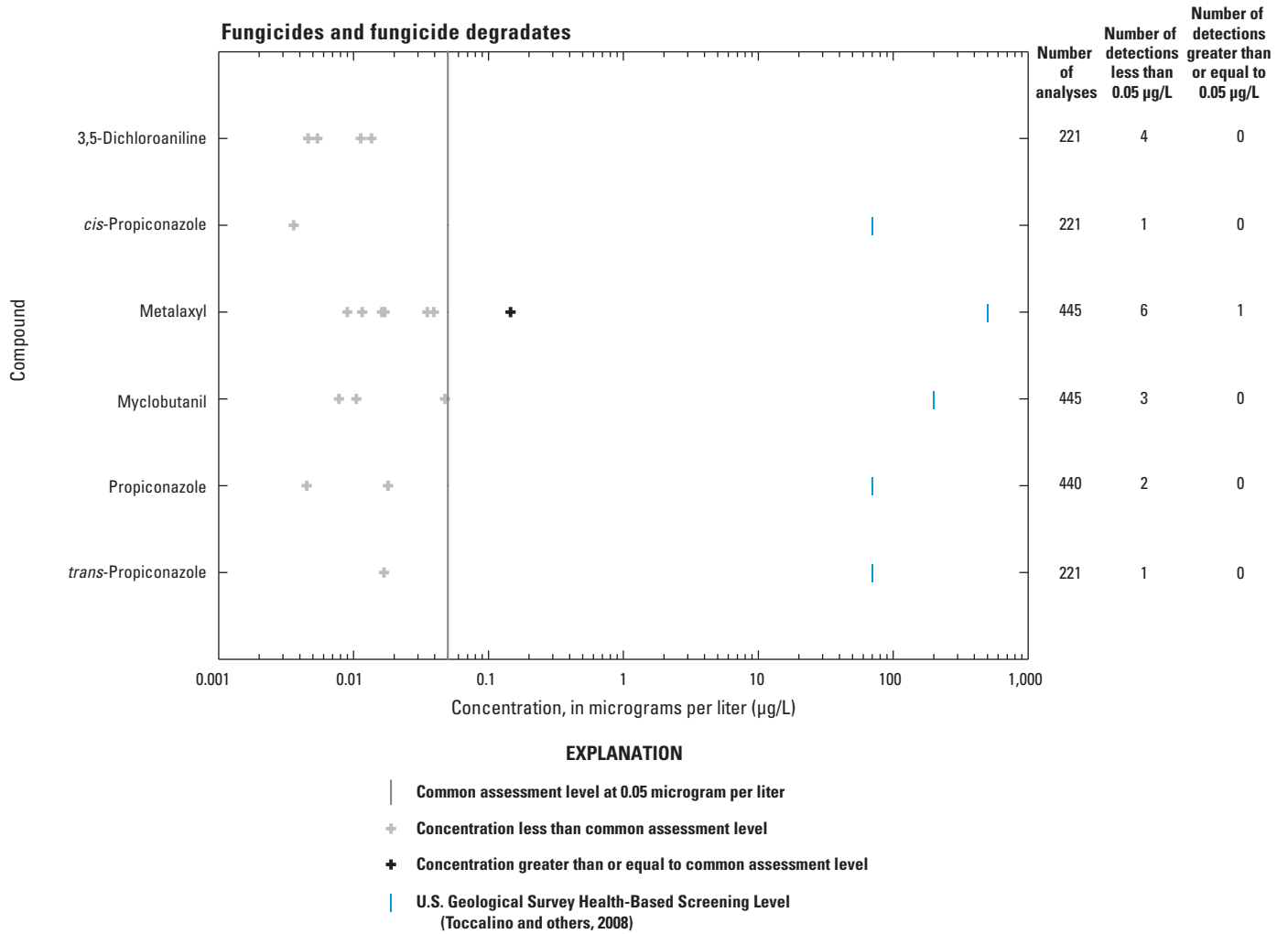


Figure 5–1. Qualified concentrations of disinfection by-products in groundwater, 2002–09.



**Figure 5–2.** Qualified concentrations of fumigant-related compounds in groundwater, 2002–09.



**Figure 5–3.** Qualified concentrations of fungicides and fungicide degradates compounds in groundwater, 2002–09.

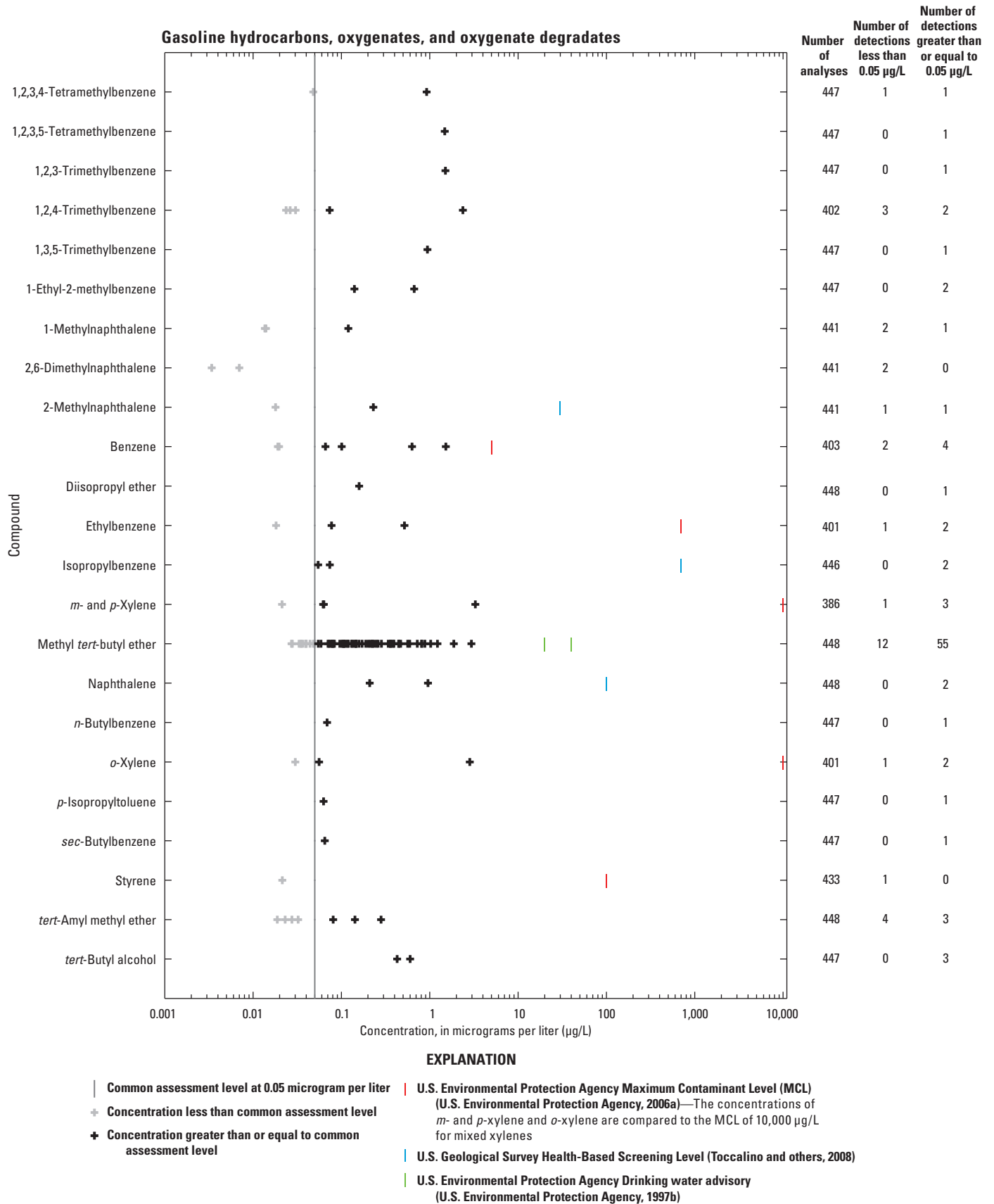


Figure 5–4. Qualified concentrations of gasoline hydrocarbons, oxygenates, and oxygenate degradates in groundwater, 2002–09.

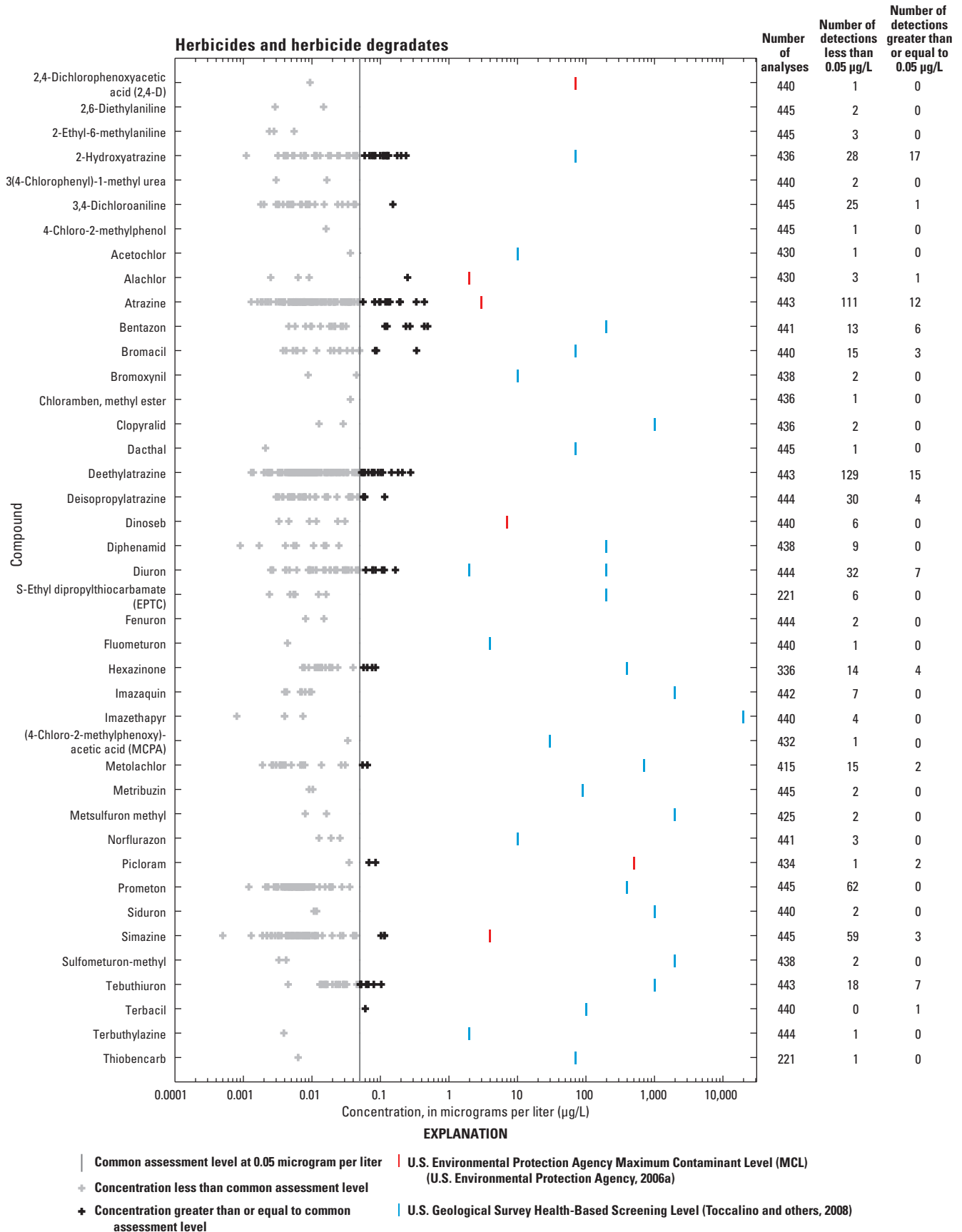


Figure 5-5. Qualified concentrations of herbicides and herbicide degradates in groundwater, 2002–09.

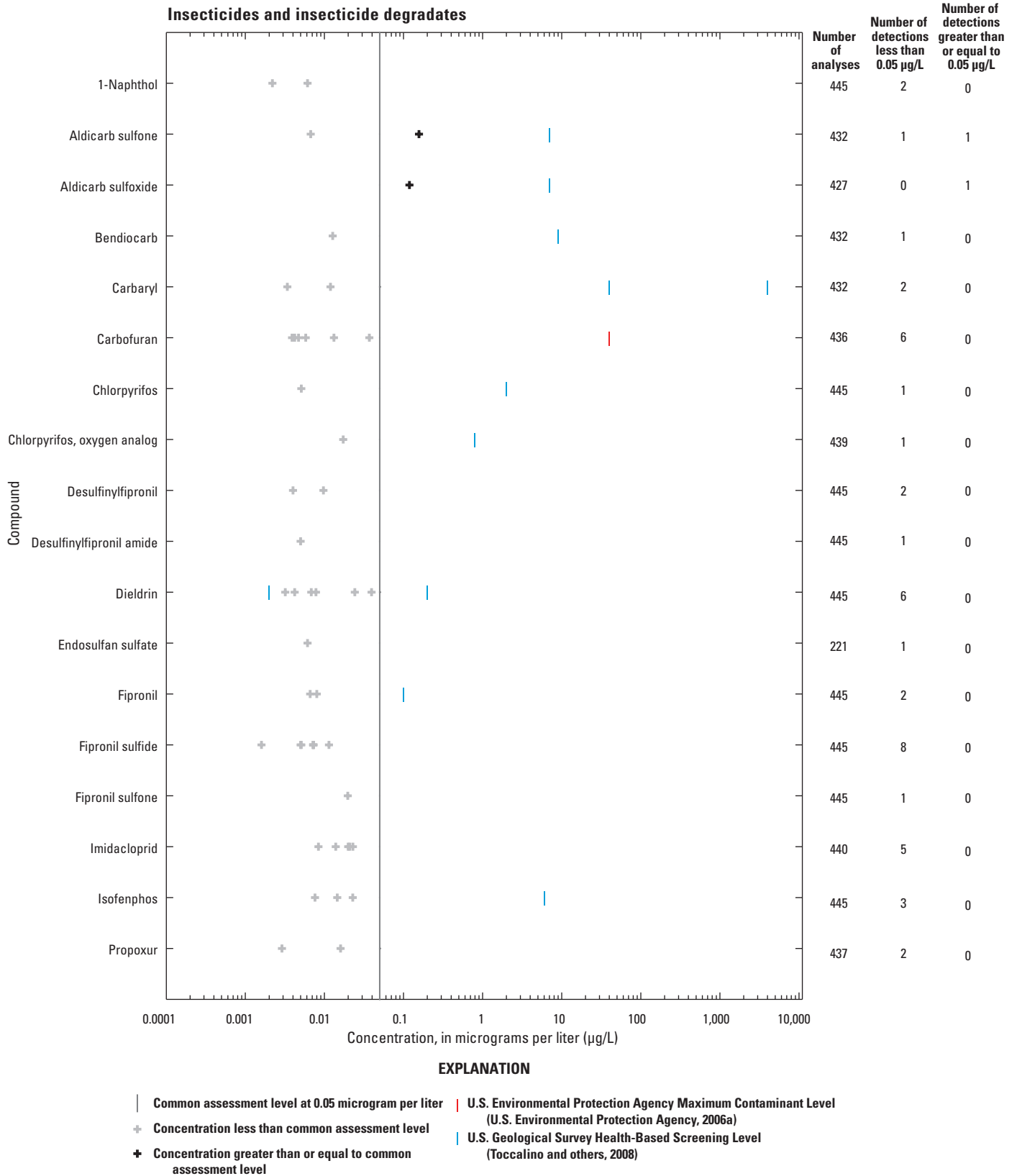
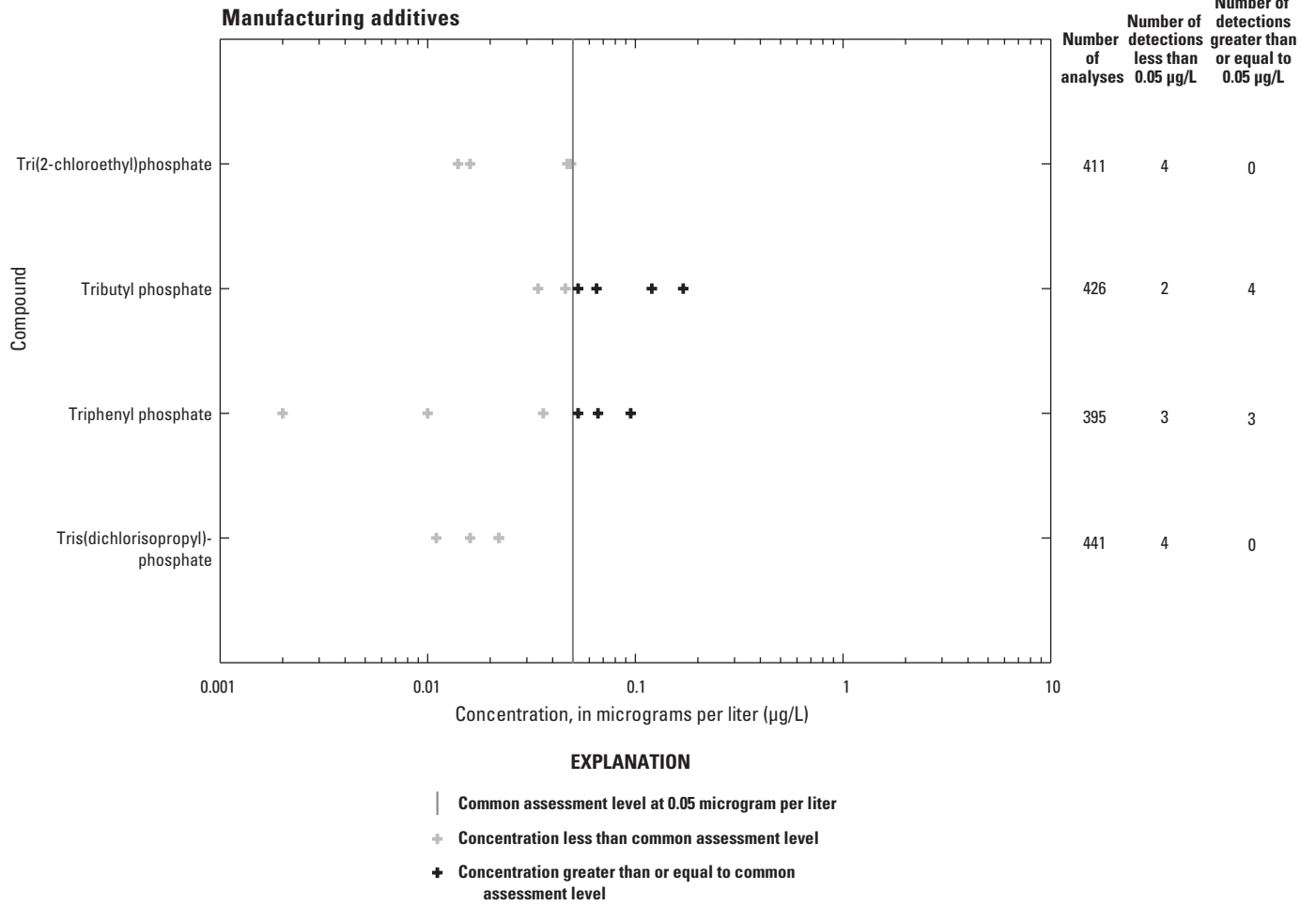
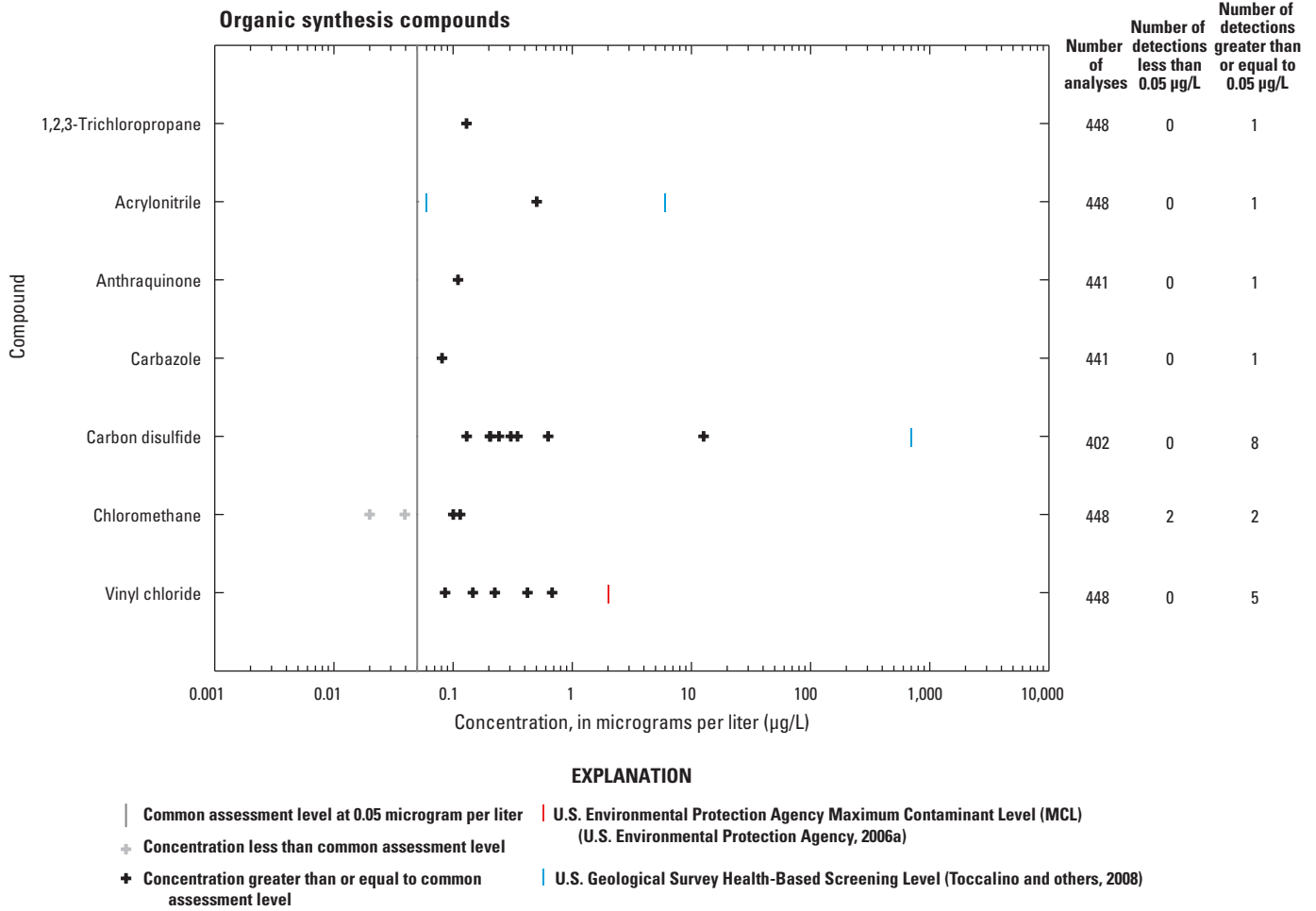


Figure 5–6. Qualified concentrations of insecticides and insecticide degradates in groundwater, 2002–09.

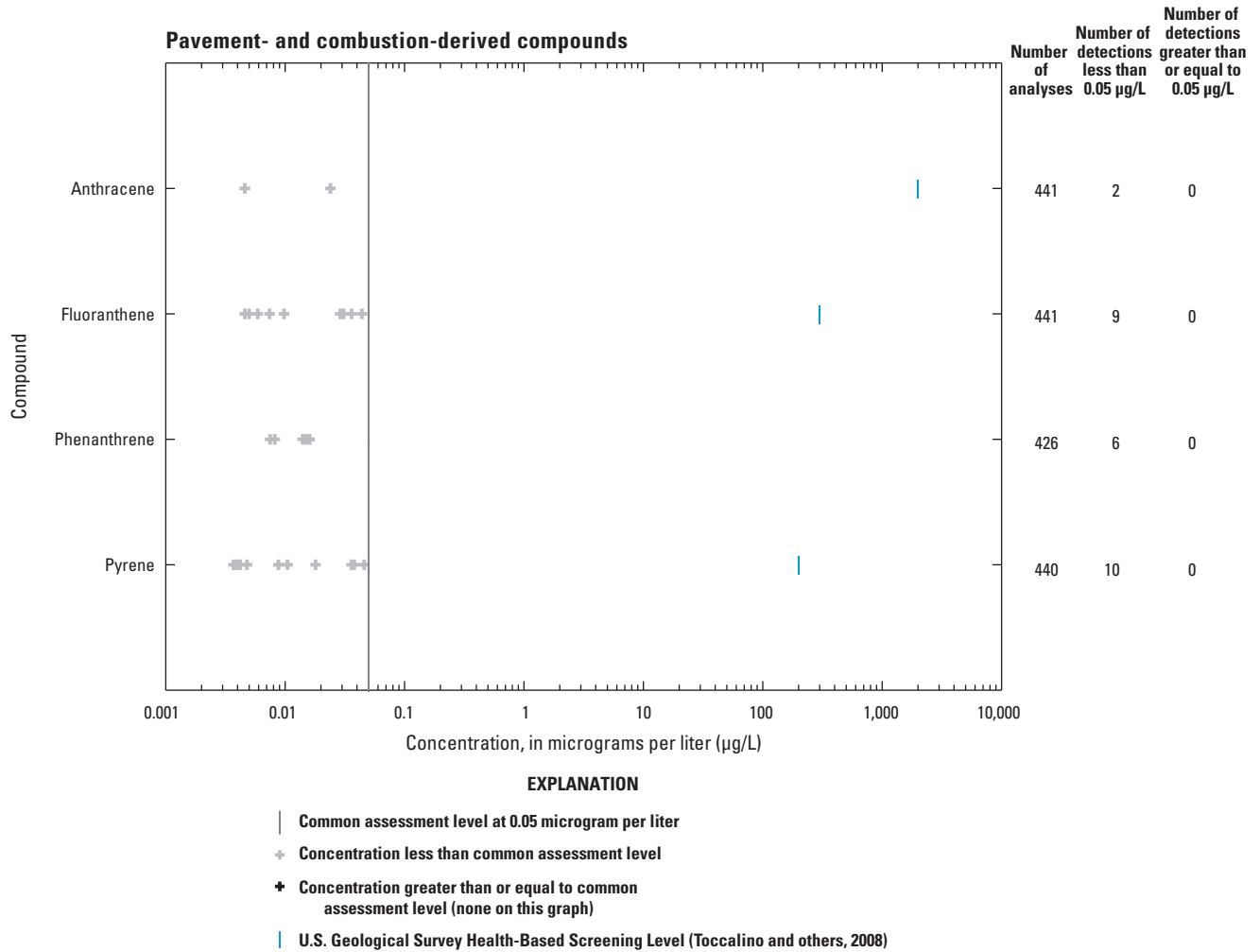




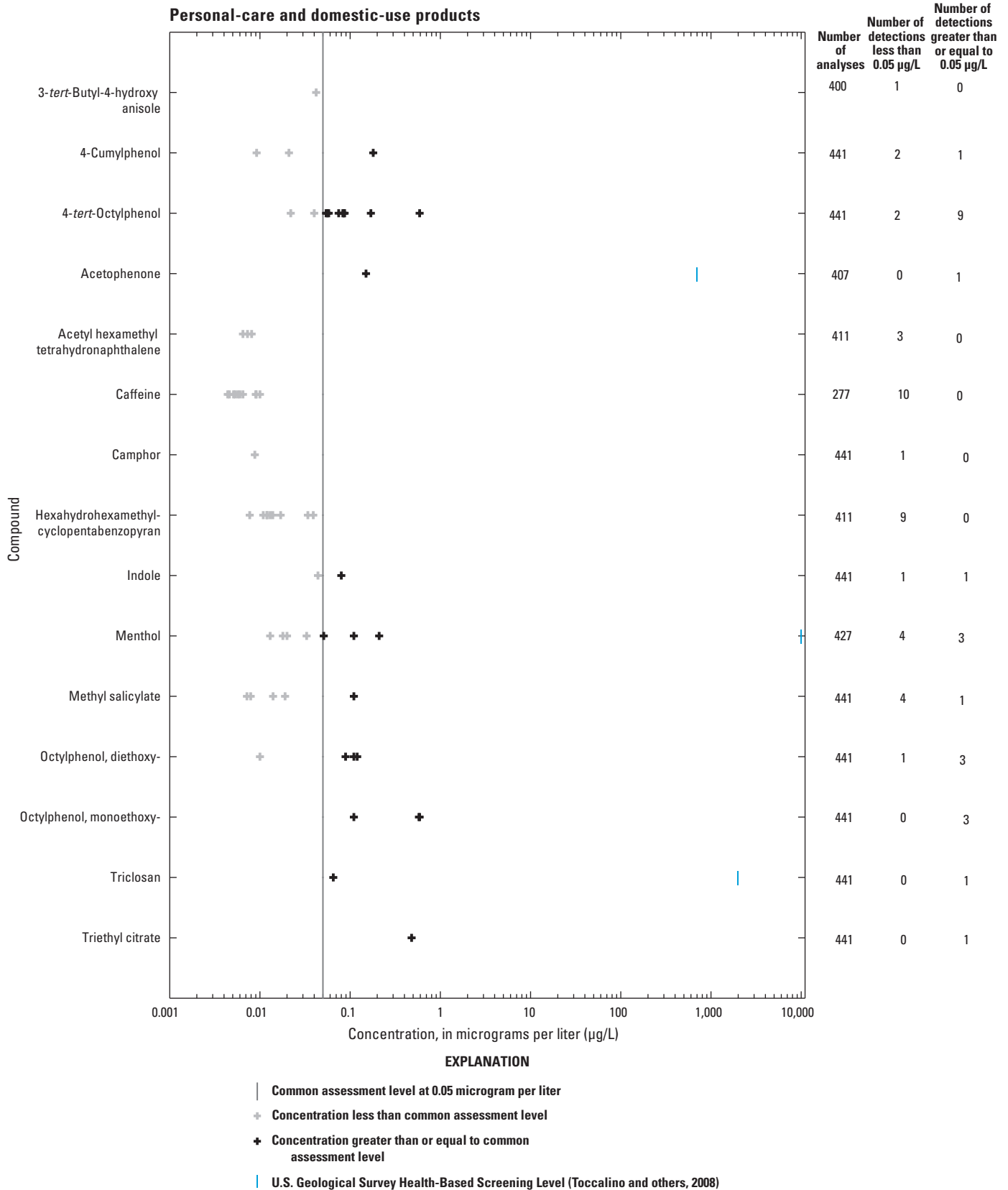
**Figure 5-7.** Qualified concentrations of manufacturing additives in groundwater, 2002-09.



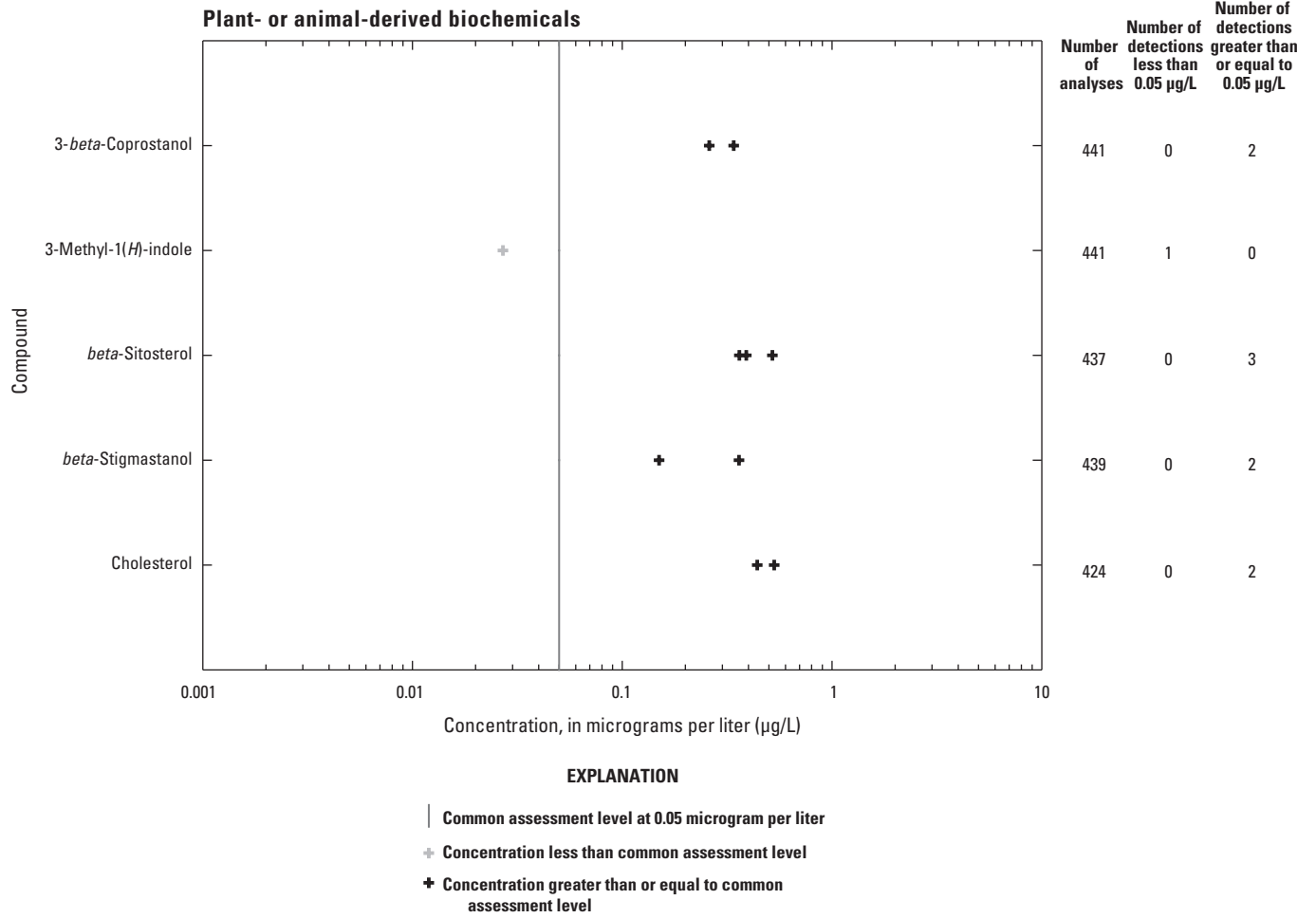
**Figure 5–8.** Qualified concentrations of organic synthesis compounds in groundwater, 2002–09.



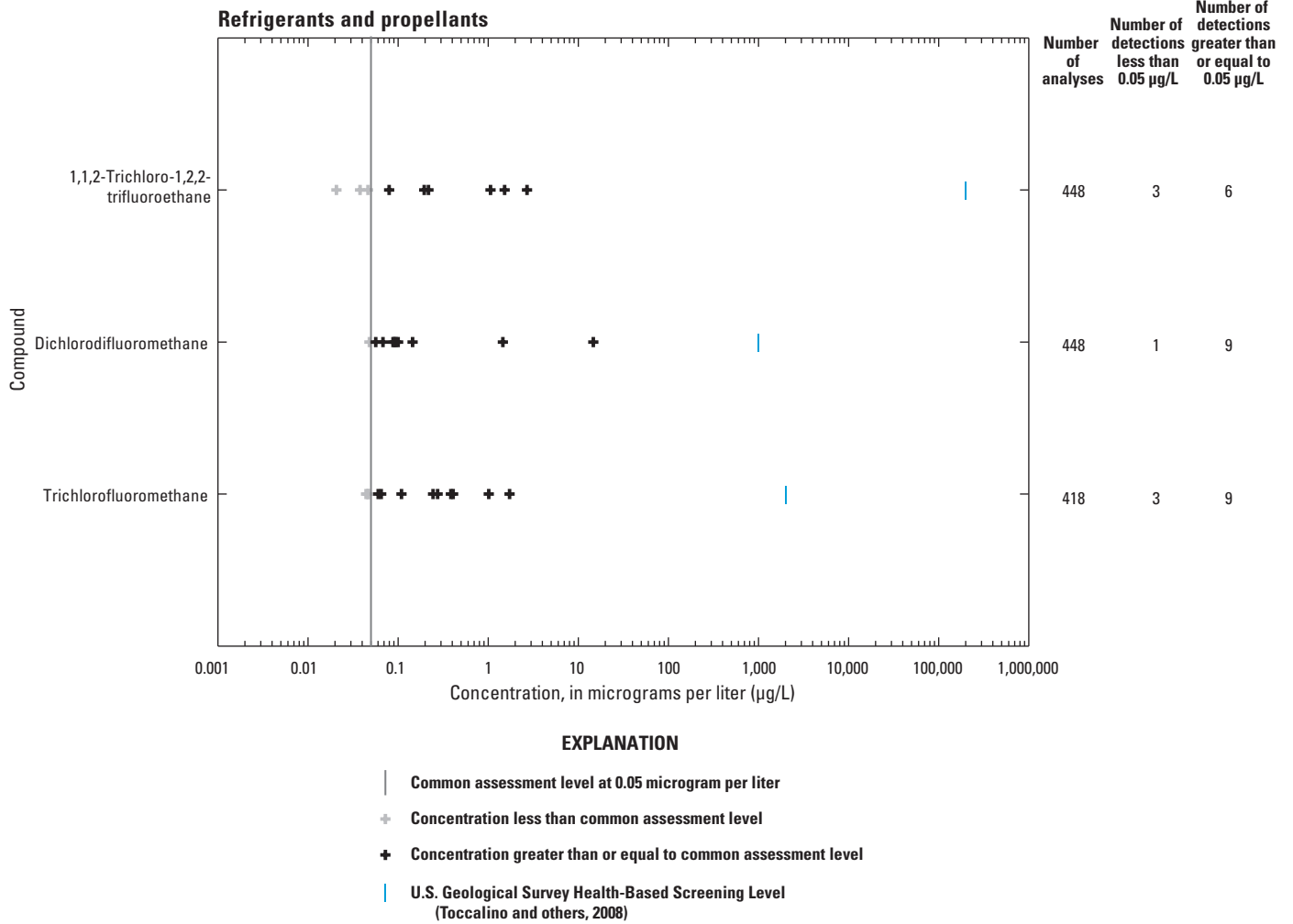
**Figure 5–9.** Qualified concentrations of pavement- and combustion-derived compounds in groundwater, 2002–09.



**Figure 5–10.** Qualified concentrations of personal-care and domestic-use products in groundwater, 2002–09.



**Figure 5–11.** Qualified concentrations of plant- or animal-derived biochemicals in groundwater, 2002–09.



**Figure 5–12.** Qualified concentrations of refrigerants and propellants in products in groundwater, 2002–09.

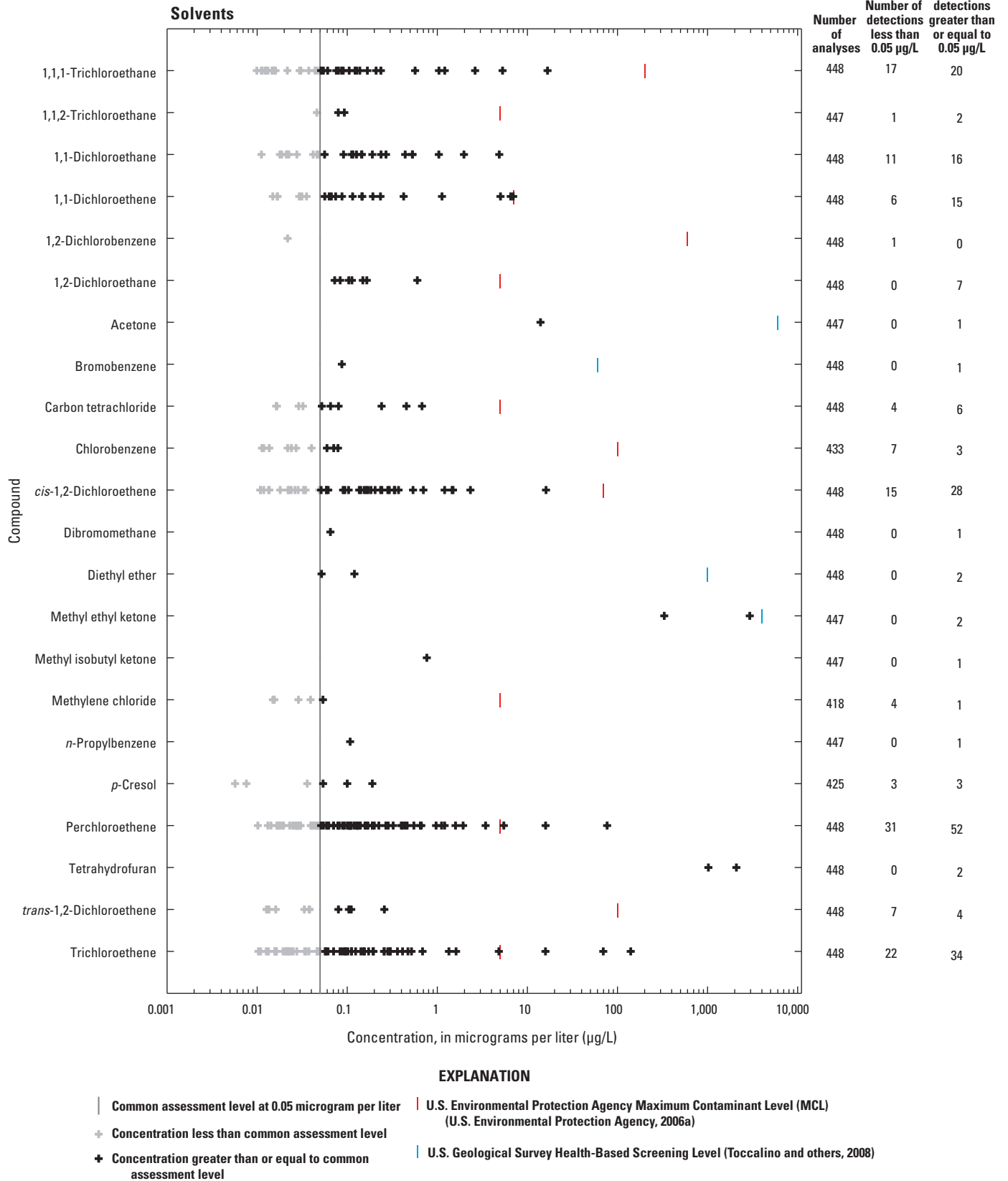


Figure 5-13. Qualified concentrations of solvents in products in groundwater, 2002-09.

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