science for a changing world

National Water-Quality Assessment Program
Source Water-Quality Assessment

Concentration Data for Anthropogenic Organic Compounds in Groundwater, Surface Water, and Finished Water of Selected Community Water Systems in the United States, 2002–10

Data Series 544

U.S. Department of the Interior
U.S. Geological Survey

Concentration Data for Anthropogenic Organic Compounds in Groundwater, Surface Water, and Finished Water of Selected Community Water Systems in the United States, 2002–10

By Janet M. Carter, James A. Kingsbury, Jessica A. Hopple, and Gregory C. Delzer

National Water-Quality Assessment Program Source Water-Quality Assessment

Data Series 544

U.S. Department of the Interior
U.S. Geological Survey

U.S. Department of the Interior
KEN SALAZAR, Secretary

U.S. Geological Survey
Marcia K. McNutt, Director

U.S. Geological Survey, Reston, Virginia: 2010

For more information on the USGS—the Federal source for science about the Earth, its natural and living resources, natural hazards, and the environment, visit http://www.usgs.gov or call 1-888-ASK-USGS

For an overview of USGS information products, including maps, imagery, and publications, visit http://www.usgs.gov/pubprod

Suggested citation:
Carter, J.M., Kingsbury, J.A., Hopple, J.A., and Delzer, G.C., Concentration data for anthropogenic organic compounds in groundwater, surface water, and finished water of selected community water systems in the United States, 2002–10: U.S. Geological Survey Data Series 544, 36 p.

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*).

National and regional assessments are ongoing in the second decade (2001–2012) 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 contaminants, the transport of those contaminants through the hydrologic system, and the potential effects of contaminants 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 contaminants 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

Contents

Figure

Tables

Conversion Factors

SI to Inch/Pound

Multiply	By	To obtain
	Length	
kilometer (km)	0.6214	mile (mi)

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

Concentrations of chemical constituents in water are given either in milligrams per liter (mg/L) or micrograms per liter (µg/L).

Acronyms and Abbreviations

<	less than
AOC	anthropogenic organic compound
BTEX	benzene, toluene, ethylbenzene, and xylenes
CWS	community water system
DEET	N,N-diethyl-*meta*-toluamide
E	estimated
GC/MS	gas chromatography-mass spectrometry
HPLC/MS	high performance liquid chromatography-mass spectrometry
LRL	laboratory reporting level
LT–MDL	long-term method detection level
NAWQA	National Water-Quality Assessment
NWQL	National Water Quality Laboratory
R	removed
SWQA	Source Water-Quality Assessment
USGS	U.S. Geological Survey
VOC	volatile organic compound

Concentration Data for Anthropogenic Organic Compounds in Groundwater, Surface Water, and Finished Water of Selected Community Water Systems in the United States, 2002–10

By Janet M. Carter, James A. Kingsbury, Jessica A. Hopple, and Gregory C. Delzer

Abstract

The National Water-Quality Assessment Program of the U.S. Geological Survey began implementing Source Water-Quality Assessments (SWQAs) in 2001 that focus on characterizing the quality of source water and finished water of aquifers and major rivers used by some of the larger community water systems in the United States. As used in SWQA studies, source water is the raw (ambient) water collected at the supply well before water treatment (for groundwater) or the raw (ambient) water collected from the river near the intake (for surface water), and finished water is the water that has been treated and is ready to be delivered to consumers. Finished-water samples are collected before the water enters the distribution system.

The primary objective of SWQAs is to determine the occurrence of more than 250 anthropogenic organic compounds in source water used by community water systems, many of which currently are unregulated in drinking water by the U.S. Environmental Protection Agency. A secondary objective is to understand recurrence patterns in source water and determine if these patterns also occur in finished water before distribution. SWQA studies were conducted in two phases for most studies completed by 2005, and in one phase for most studies completed since 2005.

Analytical results are reported for a total of 295 different anthropogenic organic compounds monitored in source-water and finished-water samples collected during 2002–10. The 295 compounds were classified according to the following 13 primary use or source groups: (1) disinfection by-products; (2) fumigant-related compounds; (3) fungicides; (4) gasoline hydrocarbons, oxygenates, and oxygenate degradates; (5) herbicides and herbicide degradates; (6) insecticides and insecticide degradates; (7) manufacturing additives; (8) organic synthesis compounds; (9) pavement- and combustion-derived compounds; (10) personal-care and domestic-use products; (11) plant- or animal-derived biochemicals; (12) refrigerants and propellants; and (13) solvents.

This report presents the analytical results of source-water samples from 448 community water system wells and 21 surface-water sites. This report also presents the analytical results of finished-water samples from 285 wells and 20 surface-water sites from community water systems. Results of quality-assurance/quality-control samples also are presented including data for equipment blanks, field blanks, source solution blanks, and replicate samples.

Introduction

In 1991, the U.S. Geological Survey (USGS) began the National Water-Quality Assessment (NAWQA) Program to (1) provide a nationally consistent description of current water-quality conditions for the 51 largest and most important aquifers and river basins across the Nation; (2) define long-term trends in water quality; and (3) identify, describe, and explain, as possible, the primary factors that affect observed water-quality conditions and trends (Gilliom and others, 1995). This information, which is obtained on a continuing basis, is made available to water managers, policy makers, and the general public to provide an improved scientific basis for evaluating the effectiveness of water-quality management programs and for predicting the likely effects of contemplated changes in land- and water-management practices. The first decade of the NAWQA Program focused on describing current water-quality conditions.

Beginning in 2001, the NAWQA Program began its second decade of intensive assessment activities, returning to 42 (14 each in 2001, 2004, and 2007, respectively) of the 51 original aquifers and river basins studied, termed Study Units. In addition to providing a description of current water-quality conditions, these studies place increased emphasis on the latter two goals of the Program—trends and understanding. In addition, a new assessment activity during the second decade of NAWQA is Source Water-Quality Assessments (SWQAs) that focus on characterizing the quality of source water and finished water of aquifers and major rivers used by some of the larger community water systems (CWSs) in the United States. As used in this study, source water is the raw (ambient) water collected at the supply well before water treatment (for groundwater) or the raw (ambient) water collected from the river near the intake (for surface water), and finished water is the water that has been treated and is ready to be delivered to consumers. Finished-water samples are collected before the water enters the distribution system. Finished water from groundwater supplies may have been blended with water from several groundwater sources, but was not blended with water from any surface-water sources. Finished water from surface-water supplies typically was not blended with any additional surface-water or groundwater sources.

SWQA studies are intended to complement drinking-water monitoring required by Federal, State, and local programs, which focus primarily on post-treatment compliance monitoring. Through SWQA studies, NAWQA is increasing its emphasis on characterizing the water quality of rivers and aquifers that are primary sources of drinking water and will allow results from other NAWQA sites to be put into context with the source of water used for water supply. Additionally, the quality of source water for a large number of compounds not regulated in drinking water by the U.S. Environmental Protection Agency also will be determined. Through SWQA studies, the USGS will continue to collaborate with other agencies and organizations involved with supplying and managing drinking water. To help accomplish this, USGS staff maintains a close working relationship with CWS personnel that are utilizing the source waters investigated.

The primary objective of SWQAs is to determine the occurrence of more than 250 primarily unregulated anthropogenic organic compounds in source water used by community water systems (Delzer and Hamilton, 2007). A secondary objective is to understand recurrence patterns in source water and determine if these patterns also occur in finished water before distribution. SWQA studies were conducted in two phases for most studies completed by 2005, and in one phase for most studies completed since 2005. The objectives of SWQA studies were met by collecting groundwater (source), surface-water (source), and finished-water samples, and analyzing these samples for anthropogenic organic compounds (AOCs).

The AOC data for the SWQAs completed during 2002–05 were presented in Carter and others (2007) and included data for the first 15 groundwater and 9 surface-water SWQAs that were sampled. Findings for the groundwater SWQAs completed during 2002–05 were presented in Hopple and others (2009), and findings for the surface-water SWQAs were presented in Kingsbury and others (2008a, 2008b). This update to Carter and others (2007) includes data for 15 additional groundwater SWQAs and 11 additional surface-water SWQAs that were completed during 2006–10. Thus, this report includes data for 30 groundwater and 20 surface-water SWQAs that were completed during 2002–10 and includes data presented in Carter and others (2007).

Before June 2005, source-water samples were analyzed for 258 AOCs. During and after June 2005, the source-water samples were analyzed for 275 AOCs, which includes all but one (fonofos, oxygen analog) of the same AOCs monitored before June 2005, plus 18 additional compounds that were not monitored previously for the SWQA studies. For SWQA studies conducted during 2002–10, samples from a subset of wells and surface-water sites also were analyzed for 3 additional pesticides and 16 pesticide degradates. Thus, source-water samples were analyzed for a total of 277 compounds before June 2005 and for a total of 294 compounds during and after June 2005. However, the total number of different AOCs analyzed for Source Water-Quality Assessment studies during 2002–10 was 295 because of the discontinuation of analyses of fonofos, oxygen analog, during June 2005.

Purpose and scope

The purpose of this report is to present concentration data for AOCs in groundwater, surface water, and finished water of CWSs sampled for SWQA studies during 2002–10. No interpretations of the concentration data are included in this report. Analytical results are reported for a total of 295 different AOCs. Specifically, this report presents the analytical results of source-water samples from 448 CWS wells and 21 surface-water sites. This report also presents the analytical results of finished-water samples from 285 wells and 20 surface-water sites from CWSs.

Results of quality-assurance/quality-control samples collected for SWQA studies during 2002–10 also are presented including data from equipment blanks, field blanks, source solution blanks, and replicate samples. Matrix spike data collected through 2006 are presented in Valder and others (2008). Data from all source-water, finished-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. If quality-control data indicated that results for environmental data were biased as a result of systematic contamination, environmental data were removed from the dataset presented in this report.

Acknowledgments

The authors thank the many CWS personnel who helped coordinate sample collection and provided permission to sample. Study Unit personnel are thanked for collecting the samples. Jack Barbash, David Bender, and Dana Kolpin are thanked for their help in compiling information for the primary use or source groups for the AOCs monitored as part of the SWQA studies.

Study Design

This section of the report describes the criteria used for selection of sampling sites for the SWQA studies. In addition, sample collection, analytical methods, and quality-assurance activities used to characterize the quality of compounds monitored are described.

Three different sampling components were used for the groundwater and surface-water SWQA studies conducted during 2002–10 (table 1). Sampling component 1 was used as the initial sampling phase for most studies conducted during 2002–05. For sampling component 1, source-water samples were collected and analyzed for all AOCs. Sampling component 2 was used as the second sampling phase for most of the studies conducted during 2002–05. During this second sampling phase, samples were collected from a subset of the wells sampled during the initial sampling phase and analyzed for those AOCs found to occur most frequently or at relatively higher concentrations during the initial sampling phase. Sampling component 3 was used for most SWQA studies conducted after 2005. For sampling component 3, source-water and finished-water samples were collected and analyzed for all AOCs. For sampling components 2 and 3, the finished-water samples were collected within a few hours or as much as 2 days after the source-water samples to account for residence time at the treatment plant.

Table 1. Description of sampling components for Source Water-Quality Assessment studies during 2002–10.

Sampling component	Description	Approximate sampling dates
1	Only source-water samples collected; analyzed for all anthropogenic organic compounds	2002–05
2	Source-water and finished-water samples collected from a subset of sites monitored during sampling component 1; analyzed for those anthropogenic organic compounds found to occur most frequently or at relatively higher concentrations during sampling component 1	2002–05
3	Source-water and finished-water samples collected; analyzed for all anthropogenic compounds	2006–10

Source-water data collected using sampling components 1 and 3 can be used to characterize the occurrence of AOCs in source water to meet the primary objective of SWQA studies. Source-water data collected using sampling component 2 would not be used to characterize the occurrence of AOCs in source water because these samples were collected at sites where AOCs were found to occur during sampling component 1 and were analyzed for AOCs that occurred frequently or at relatively higher concentrations during sampling component 1, and thus are not representative of general occurrence. Source-water and finished-water samples collected during sampling components 2 and 3 can be used to meet the secondary objective of SWQA studies, which is to understand recurrence patterns of AOCs in source water and determine if these patterns also occur in finished water before distribution.

Selection of Groundwater Sites

A total of 30 groundwater SWQAs were conducted and completed (fig. 1) and the source water from a total of 448 wells were sampled during 2002–10 (table 2). A total of 285 finished-water samples were collected during 2002–10.

Sixteen SWQAs were completed using two sampling phases (components 1 and 2), which were used for most SWQA studies conducted during 2002–05. These 16 SWQAs represent 14 NAWQA Study Units. Two of these Study Units—Georgia-Florida Coastal Plain (GAFL; map numbers 6 and 7 on figure 1) and Upper Mississippi River Basin (UMIS; map numbers 27 and 28 on figure 1)—had two SWQA studies (table 2). For one of these 16 SWQA studies (South Platte River Basin), source-water and finished-water samples were not collected during the second phase because AOCs were detected infrequently and at relatively low concentrations in source water during the initial sampling phase. For each groundwater SWQA, about 15 CWS wells were selected, for a total of 237 wells sampled for source water using a two-phase approach. Source water and finished water were monitored as part of sampling component 2 for about 85 of the 237 CWS wells.

Fourteen SWQAs were completed using a single sampling phase (component 3), which was used for most SWQA studies conducted after 2005. These 14 SWQAs represent 13 NAWQA Study Units. One of these Study Units—Southern Florida (SOFL; map numbers 23 and 24 on figure 1)—had two SWQA studies (table 2). A total of 211 wells were sampled for source and finished water through 2010 using a single sampling phase.

The selection process for CWS wells considered several criteria. The wells selected withdraw water from a principal aquifer or system (table 2), and groundwater represents a substantial portion of drinking water in the area. Additionally, groundwater used by the selected CWSs potentially was vulnerable to anthropogenic contamination because of large groundwater withdrawal rates from the aquifer and the proximity of wells to urban areas. Finally, the wells sampled fit into a national network of wells that collectively cover a variety of environmental land-use settings such as agriculture, urban, and mixed.

Within an SWQA study area, the highest producing wells typically were selected for sampling because these wells have the largest contributing areas, which may increase the potential for contamination. Annual production data obtained from

Table 2. Principal aquifers or aquifer systems sampled for groundwater Source Water-Quality Assessment studies during 2002–10.

Map number (shown on figure 1)	Source Water-Quality Assessment study (Study Unit abbreviation)	State(s) in which SWQA was located	Number of wells sampled	Principal aquifer[a] or system in which SWQA was conducted	Sampling component used for study (table 1)
1	Acadian-Pontchartrain Drainages (ACAD)	Louisiana	15	Coastal Lowlands aquifer system	3
2	Central Arizona Basins (CAZB)	Arizona	13	Basin and Range basin-fill aquifers	3
3	Central Columbia Plateau/Yakima River Basin (CCYK)[b]	Washington	15	Columbia Plateau basin-fill and basaltic-rock aquifers	1 and 2
4	Connecticut, Housatonic, and Thames River Basins (CONN)[b]	Connecticut	15	Glacial deposits aquifer system	1 and 2
5	Eastern Iowa Basins (EIWA)	Iowa	15	Cambrian-Ordovician aquifer system	3
6	Georgia-Florida Coastal Plain (GAFL)[b]	Florida	15	Floridan aquifer system (unconfined unit)	1 and 2
7	Georgia-Florida Coastal Plain (GAFL)[b]	Florida	15	Floridan aquifer system (semiconfined unit)	1 and 2
8	Great Salt Lake Basins (GRSL)	Utah	16	Basin and Range basin-fill aquifers	3
9	High Plains Regional Groundwater Study (HPGW)[b]	Nebraska	15	High Plains aquifer	1 and 2
10	Long Island-New Jersey Coastal Drainages (LINJ)	New York	15	Northern Atlantic Coastal Plain aquifer system	3
11	Lower Illinois River Basin (LIRB)	Illinois	16	Sand and gravel aquifers (glaciated regions)	3
12	Mississippi Embayment (MISE)	Mississippi, Tennessee	15	Mississippi embayment aquifer system	1 and 2
13	New England Coastal Basins (NECB)	New Hampshire	16	New England crystalline-rock aquifers	3
14	Nevada Basin and Range (NVBR)[b]	Nevada	15	Basin and Range basin-fill aquifers	1 and 2
15	Potomac River Basin and Delmarva Peninsula (PODL)[b]	Maryland, Virginia	15	Piedmont and Blue Ridge crystalline-rock aquifers	1 and 2
16	Puget Sound Basin (PUGT)	Washington	15	Puget Sound aquifer system	1 and 2
17	Rio Grande Valley (RIOG)[b]	New Mexico	15	Rio Grande aquifer system	3
18	Sacramento River Basin (SACR)	California	15	Central Valley aquifer system	3
19	Santa Ana Basin (SANA)	California	15	California Coastal Basin aquifers	3
20	San Joaquin-Tulare Basins (SANJ)[b]	California	15	Central Valley aquifer system	1 and 2
21	Santee River Basin and Coastal Drainages (SANT)	South Carolina	15	Piedmont and Blue Ridge crystalline-rock aquifers	3
22	South-Central Texas (SCTX)[b]	Texas	15	Edwards-Trinity aquifer system	1 and 2
23	Southern Florida (SOFL)	Florida	15	Surficial aquifer system	3
24	Southern Florida (SOFL)	Florida	15	Biscayne aquifer	3
25	South Platte River Basin (SPLT)[b]	Colorado	12	Denver Basin aquifer system	1[c]
26	Trinity River Basin (TRIN)[b]	Texas	15	Coastal Lowlands aquifer system	1 and 2
27	Upper Mississippi River Basin (UMIS)[b]	Minnesota, Wisconsin	15	Glacial deposits aquifer system	1 and 2
28	Upper Mississippi River Basin (UMIS)[b]	Minnesota, Wisconsin	15	Cambrian-Ordovician aquifer system (Prairie du Chien-Jordan aquifer)	1 and 2
29	Upper Snake River Basin (USNK)	Idaho	15	Snake River Plain basin-fill and basaltic-rock aquifers	3
30	White and Great and Little Miami River Basins (WHMI)[b]	Ohio	15	Glacial deposits aquifer system	1 and 2
Total number of wells sampled			**448**		

[a]Principal aquifer from U.S. Geological Survey (2003).

[b]Data for Source Water-Quality Assessment was included in Carter and others (2007).

[c]No source-water or finished-water samples from this site were collected during sampling component 2.

the CWSs were used to characterize withdrawals for the CWS 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. The top quartile of individual CWS wells or pumping centers in a study area was characterized, and 15 CWS wells randomly were selected from those in the top quartile. For areas where the top quartile did not contain enough wells or pumping centers for a random selection of 15 wells to occur, a larger group of wells (for example, the upper one-half) was used. Wells sampled were at least 1 kilometer (km) apart to ensure that the contributing areas for wells did not overlap and to be consistent with other NAWQA studies (for example, Toccalino and others, 2010). The type of water treatment used by the CWSs was not considered in the selection process.

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. CWS wells with strong connections to streams (under the influence of surface water) were not used. 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 from these types of wells does not represent recharge from the land surface.

Selection of Surface-Water Sites

A total of 20 surface-water SWQAs were conducted during 2002–10 (table 3, fig. 1), with a total of 21 source-water sites sampled and 20 finished-water sites sampled. Water quality from surface-water SWQAs was monitored in 12 NAWQA Study Units as part of sampling component 1 and in 8 Study Units as part of sampling component 3 (table 3). For most surface-water SWQAs conducted during 2002–05, one site was selected for each SWQA and sampled monthly for about 1 year as part of sampling component 1. During the second sampling phase (sampling component 2), source water and finished water were sampled for 11 of the 12 surface-water SWQAs monitored using sampling component 1; finished-water samples were not collected from the South Platte River Basin Study Unit during this second phase because relatively few AOCs were detected during the initial sampling phase for this SWQA. For most SWQAs conducted after 2005, source-water and finished-water samples were collected for eight

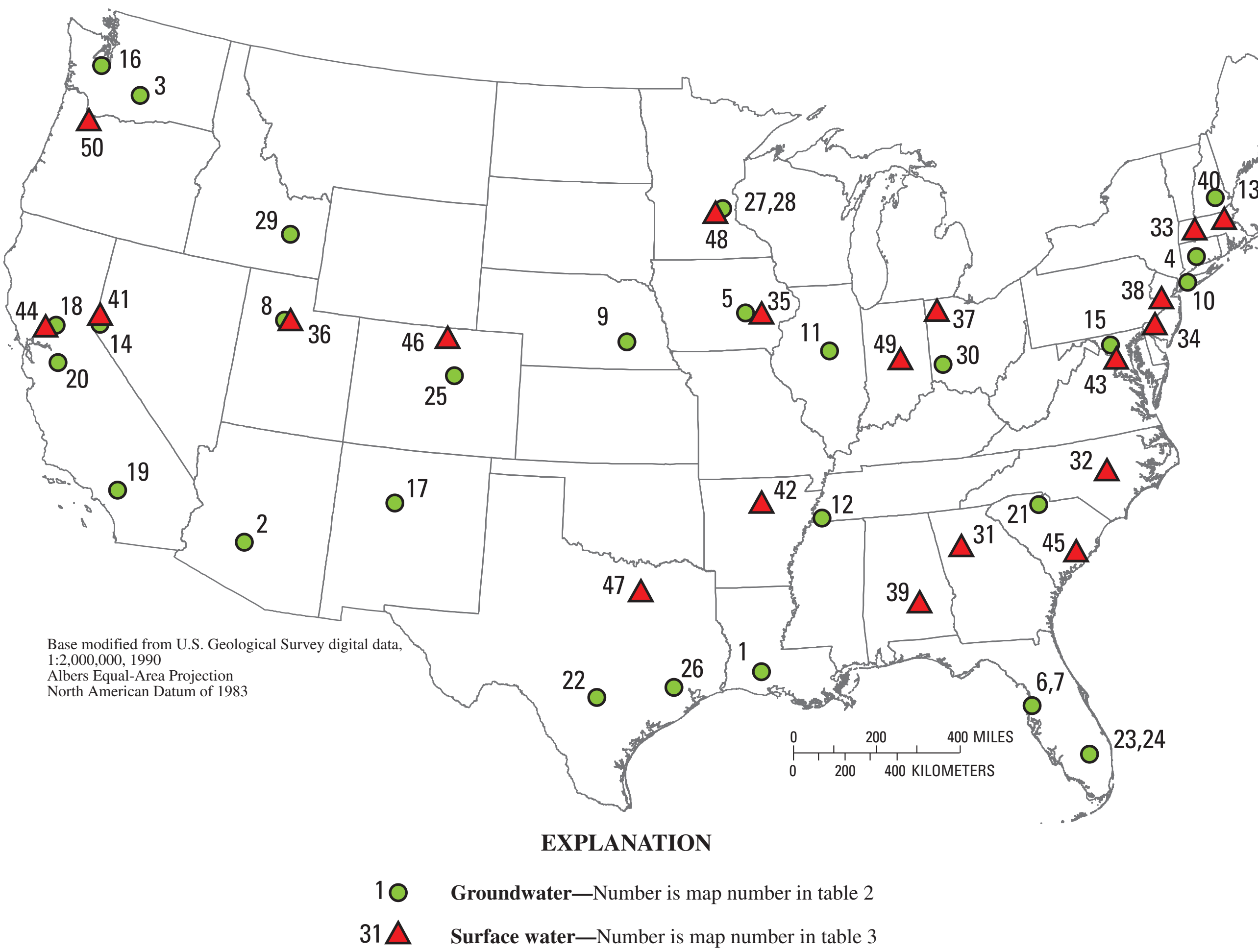

Figure 1. Location of Source Water-Quality Assessment studies for which samples were collected during 2002–10.

Table 3.. Rivers sampled for surface-water Source Water-Quality Assessment studies during 2002–10.

Map number (shown on figure 1)	Source Water-Quality Assessment study (Study unit abbreviation)	River	System size[a]	Sampling component used for study (table 1)
31	Apalachicola-Chattahoochee-Flint River Basins (ACFB)[b]	Chattahoochee River, Georgia	Very large	1 and 2
32	Albemarle-Pamlico Drainage Basin (ALBE)[b]	Neuse River, North Carolina	Large	1 and 2
33	Connecticut, Housatonic, and Thames River Basins (CONN)[b]	Running Gutter Creek, Massachusetts	Small	1 and 2
34	Delaware River Basin (DELR)	Schuylkill River, Pennsylvania	Very large	3
35	Eastern Iowa Basins (EIWA)	Iowa River, Iowa	Large	3
36	Great Salt Lake Basins (GRSL)	Provo River, Utah	Very large	3
37	Lake Erie-Lake Saint Clair Drainages (LERI)	Maumee River, Ohio	Large	3
38	Long Island-New Jersey Coastal Drainages (LINJ)	Raritan River, New Jersey	Very large	3
39	Mobile River Basin (MOBL)	TallaPoosa River, Alabama	Very large	3
40	New England Coastal Basins (NECB)	Merrimack River, Massachusetts	Very large	3
41	Nevada Basin and Range (NVBR)[b]	Truckee River, Nevada	Very large	1 and 2
42	Ozark Plateaus (OZRK)	White River, Arkansas	Large	3
43	Potomac River Basin and Delmarva Peninsula (PODL)[b]	Potomac River, Maryland	Very large	1 and 2
44	Sacramento River Basin (SACR)	Sacramento River, California	Large	1 and 2
45	Santee River Basin and Coastal Drainages (SANT)	Back River, South Carolina	Very large	1 and 2
46	South Platte River Basin (SPLT)[b]	Cache la Poudre River, Colorado	Very large	1[c]
47	Trinity River Basin (TRIN)[b]	Elm Fork Trinity River, Texas	Very large	1 and 2
48	Upper Mississippi River Basin (UMIS)	Mississippi River, Minnesota	Very large	1 and 2
49	White and Great and Little Miami River Basins (WHMI)[b]	White River, Indiana	Very large	1 and 2
50	Willamette Basin (WILL)[b]	Clackamas River, Oregon	Large	1 and 2

[a]System size is defined by U.S. Environmental Protection Agency (2010) as follows: small, serving 501 to 3,300 people; large, serving 10,001 to 100,000 people; and very large, serving more than 100,000 people.

[b]Data for Source Water-Quality Assessment was included in Carter and others (2007).

[c]No source-water or finished-water samples from this site were collected during phase 2.

NAWQA Study Units as part of sampling component 3 (table 3). Similar to sampling component 1, one site was selected for each SWQA and sampled monthly for about 1 year using sampling component 3; however, for one SWQA (Long Island-New Jersey Coastal Drainages; map number 38 on figure 1), two different source-water sites and two different finished-water sites were sampled.

Several criteria were used in selecting a surface-water CWS site for SWQA monitoring. Source-water sites were selected on free-flowing stream reaches rather than on reservoirs to remain consistent with and to be able to compare results with other surface-water sites sampled by the NAWQA Program. In some cases, reservoirs were upstream from the surface-water CWS sites, but the closest reservoir was about 7 km upstream from the CWS intake. The median distance between the CWS intake and an upstream reservoir was about 40 km, and the farthest reservoir was more than 100 km upstream from the intake. Additionally, CWSs selected for this study were single-source systems, with little or no blending of other source waters. Land use in the watershed and the type of water treatment used by the CWSs were not considerations in site selection.

The surface-water CWSs sampled represent a range in size (table 3) and are fairly well distributed across the United States (fig. 1). Nineteen of the 20 CWSs are categorized as large or very large water systems, meaning that they provide water to more than 10,001 and 100,001 people, respectively (U.S. Environmental Protection Agency, 2010). One site, Running Gutter Creek, Massachusetts (map number 33 on figure 1), is a small CWS that serves fewer than 3,300 people.

Compounds Monitored

The 295 AOCs monitored for SWQA studies during 2002–10 were categorized into the following 13 compound groups based on their primary use or source (table 4): (1) disinfection by-products; (2) fumigant-related compounds; (3) fungicides and fungicide degradates; (4) gasoline hydrocarbons, oxygenates, and oxygenate degradates; (5) herbicides and herbicide degradates; (6) insecticides and insecticide degradates; (7) manufacturing additives; (8) organic synthesis compounds; (9) pavement- and combustion-derived compounds; (10) personal-care and domestic-use products; (11) plant- or animal-derived biochemicals; (12) refrigerants and propellants; and (13) solvents. Use information for the compounds analyzed for SWQA studies is presented in Appendix 1.

Sample Collection and Analytical Methods

Groundwater, surface-water, and quality-control samples were collected using established USGS protocols (Koterba and others, 1995; U.S. Geological Survey, variously dated). Groundwater samples were collected at the wellhead before any treatment such as chlorination. Surface-water samples were collected approximately 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 at a single depth integrated point as close as practical to the drinking-water intake and processed following standard USGS sampling protocols (U.S. Geological Survey, variously dated).

Finished-water samples associated with each groundwater and surface-water source-water sample were collected following all of the treatment steps before the water entered the water treatment plants' distribution systems. These samples typically were collected where samples are collected for compliance monitoring. The finished-water samples were collected within a few hours or as much as 2 days after the source-water samples to try to account for the residence time in the treatment plant based on information provided by treatment plant personnel. Finished-water samples typically contain free chlorine, which has been documented to degrade certain organic compounds that may be present in the water samples (Munch, 1995); therefore, a dechlorination reagent (ascorbic acid) and, for certain samples, pH buffers (Trizma) were added to finished-water samples during sample collection to stabilize them before analyses. The effect of these dechlorination reagents on the laboratory analysis was evaluated, and results indicated that analytical methodologies were not affected by the addition of these reagents (Mark Sandstrom, U.S. Geological Survey National Water Quality Laboratory, written commun., 2007). Finished-water sample results are not necessarily representative of drinking-water quality at the tap because samples were collected before distribution and thus do not account for the additional contact time that the water has with disinfectants in the distribution system.

Samples were analyzed using six USGS approved analytical schedules at the USGS National Water Quality Laboratory (NWQL) in Denver, Colorado, and described by Zaugg and others (1995), Lindley and others (1996), Connor and others (1998), Furlong and others (2001), Sandstrom and others (2001), Zaugg and others (2002), and Madsen and others (2003). These methods include gas chromatography-mass spectrometry (GC/MS) and high performance liquid chromatography-mass spectrometry (HPLC/MS) analytical techniques. Samples collected for volatile organic compound (VOC) analyses using schedules 2020 and 4024 (Appendix 1) were chilled upon collection. Samples collected for analyses using schedule 2020 also were preserved using 1:1 hydrochloric acid. VOC sample sets were analyzed by purge and trap GC/MS (Connor and others, 1998; Rose and Sandstrom, 2003). Samples for analyses of pesticides and other semi-volatile 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 were then eluted with a solvent and the extracts were analyzed by either GC/MS or HPLC/MS methods (Zaugg and others, 1995; Lindley and others, 1996; Furlong and others, 2001; Sandstrom and others, 2001; Zaugg and others, 2002; Madsen and others, 2003). During June 2005, schedule 2003 was replaced by schedule 2033, which includes all but one (fonofos, oxygen analog) of the same pesticides (fungicides, herbicides, and insecticides) monitored before June 2005, plus 18 additional compounds that were not monitored previously for the SWQA studies (Appendix 1). At a subset of sites, an additional sample was collected for the analysis of 3 herbicides and 16 herbicide degradates. These additional samples were analyzed using HPLC/MS by the Organic Geochemistry Research Group Laboratory, in Lawrence, Kansas (Lee and Strahan, 2003).

AOC concentrations detected below the lowest daily standard, or for information-rich methods, concentrations detected below the long-term method detection level (LT–MDL), are reported as estimated concentrations (Childress and others, 1999). The laboratory report level (LRL) generally is equal to twice the yearly determined LT–MDL (Childress and others, 1999). The LT–MDL is a detection level derived by determining the standard deviation or a minimum of 24 MDL spike-sample measurements throughout an extended time. The LT–MDL data are collected on a continuous basis to assess year-to-year variations in the LT–MDL. The chance of falsely reporting a concentration at or greater than the LT–MDL for a sample that did not contain the analyte is predicted to be less than or equal to 1 percent (Childress and others, 1999). Also, at low concentrations, especially concentrations less than the LRL, the variability of detection is high, false negatives are more likely, and greater variability in reported concentrations is expected (Martin, 2002). Concentrations greater than the LRL sometimes are reported as estimated

Table 4. Primary use or source groups for compounds analyzed for groundwater and surface-water Source Water-Quality Assessment studies, 2002–10.

[BTEX: benzene, toluene, ethylbenzene, and xylenes]

Primary use or source group	Description	Number of compounds in group for samples analyzed	
		Before June 2005	During and after June 2005
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	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	9
Fungicides and fungicide degradates	Pesticides that are used to kill unwanted fungi.	7	11
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 compounds are among those present in the greatest proportions in gasoline. Oxygenates such as methyl *tert*-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	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).	82	88
Insecticides and insecticide degradates	Pesticides designed to kill unwanted insects (insecticides) and compounds produced from the transformation of the parent insecticide following application (degradates).	51	58
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.	7	7
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	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	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.	26	26
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	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	3
Solvents	Compounds that are used to dissolve other substances. Two of the more common solvents are trichloroethene (TCE) and perchloroethene (PCE).	33	33
Total number of compounds[a]		**277**	**294**

[a]The total number of different anthropogenic organic compounds analyzed for Source Water-Quality Assessment studies during 2002–10 was 295.

concentrations for some AOCs because of the variability in the analytical method, poor recovery, or by loss processes such as water-matrix interferences that result in false-negative errors. Concentrations are censored and reported as less than (<) the LRL when the compound was not detected.

Quality Assurance

Quality-assurance/quality-control samples collected for SWQA studies include equipment blanks, field blanks, source solution blanks, and replicate samples. 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 before the environmental samples are collected. Equipment blanks are used to evaluate the cleanliness of sampling equipment. Field blanks are collected 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, and the atmosphere. Source solution blanks are used to determine the presence or absence of compounds in the water used to clean equipment and process field blanks. The various blank samples also provide information on contamination during shipment. Replicate samples measure the combined precision of sampling and laboratory analyses. Matrix spike samples, which provide information about recoveries of organic compounds, also were collected for SWQA studies and were reported for 2004 to 2006 by Valder and others (2008).

Data from all source-water, finished-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 the quality-control data along with the associated environmental data is important because the relatively small number of samples collected in each study area generally is not adequate to characterize the full magnitude of potential bias on an individual SWQA basis. 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. These quality-control reviews were completed on an annual basis. If quality-control data indicated that results for environmental data were biased as a result of systematic contamination, environmental data were removed from the dataset presented in this report by coding concentrations with an “R.”

Data for seven AOCs were removed from the dataset presented in this report because of systematic contamination or analytical variability. 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 for this report by coding concentrations with an “R.” 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; thus, concentrations for DEET were removed for this report by coding concentrations with an “R.” 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 the quality of data for benzophenone, isophorone, and para-nonylphenol is not fully understood, concentrations for these three compounds also were removed for this report by coding concentrations with an “R.” 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 for this report by coding concentrations with an “R.”

For compounds detected in 50 percent or more of an individual Study Unit’s field blank samples, all environmental and quality-control data for that Study Unit were removed for this report by coding concentrations with an “R.” After these concentrations were removed, compounds detected in 5 percent or more of the 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<” in the remark columns and by changing the concentration to the highest blank concentration.

Concentration Data

Concentration data for the AOCs are presented in Appendix 2 for the 30 groundwater SWQAs and in Appendix 3 for the 20 surface-water SWQAs. The quality-assurance/quality-control data associated with the groundwater and surface-water SWQAs also are presented in Appendixes 2 and 3, respectively. The concentration data are presented in two formats: (1) Microsoft Excel spreadsheets, and (2) tab-delimited text files. The concentration data are presented by the primary use or source groups as defined in table 4. Concentrations for each of the 13 groups are presented either as a separate worksheet within the Excel spreadsheets, or as individual files for the tab-delimited text files.

Data are presented within each worksheet or text file in a similar order. First, the source-water (groundwater or surface-water) and finished-water samples are presented (sample type: regular), followed by quality-assurance/quality-control samples (sample types: equipment blanks, field blanks, source solution blanks, and replicates). The sample medium indicates whether the regular sample was of groundwater (source water), surface water (source water), or finished water and whether the quality-assurance/quality-control samples were associated with groundwater (source water), surface water (source water), or finished water.

The concentrations presented in Appendixes 2 and 3 are not rounded; concentrations are presented as received from the laboratories, with the following exceptions: (1) concentrations for benzophenone, bisphenol A, isophorone, DEET, para-nonylphenol (total), pentachlorophenol, and phenol were removed by coding concentrations with an “R” in the remark columns; (2) for compounds detected in 50 percent or more of an individual Study Unit’s field blank samples, all environmental and quality-control data for that Study Unit were removed for this report by coding concentrations with an “R,” and after removal of those data; (3) compounds detected in 5 percent or more of all 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<” in the remark columns and by changing the concentration to the highest blank concentration. The remark columns indicate whether a concentration was too low to be quantified (reported as a less than (<) value), censored (C), estimated (E), or removed (R).

References Cited

Agency for Toxic Substances and Disease Registry (ATSDR), 1992a, Toxicological profile for 1,2,3-trichloropropane, accessed July 30, 2010, at *http://www.atsdr.cdc.gov/toxprofiles/tp57.html*.

Agency for Toxic Substances and Disease Registry (ATSDR), 1992b, Toxicological profile for 2-hexanone, accessed July 30, 2010, at *http://www.atsdr.cdc.gov/toxprofiles/tp44.html*.

Barbash, J.E., and Reinhard, M., 1989, Abiotic dehalogenation of 1,2-dichloroethane and 1,2-dibromoethane in aqueous solution containing hydrogen sulphide: Environmental Science and Technology, v. 23, no. 11, p. 1,349–1,358.

Bender, D.A., Zogorski, J.S., Halde, M.J., and Rowe, B.L., 1999, Selection procedure and salient information for volatile organic compounds emphasized in the National Water-Quality Assessment Program: U.S. Geological Survey Open-File Report 99–182, 32 p.

Bradley, P.M., Chapelle, F.H., and Landmeyer, J.E., 2001, Effect of redox conditions on MTBE biodegradation in surface water sediments: Environmental Science and Technology, v. 35, no. 23, p. 4,643–4,647.

Budavari, Susan, ed., 1989, The Merck Index (11th ed.): Rahway, N.J., Merck and Company, Inc. [variously paged].

Budavari, Susan, ed., 1996, The Merck Index (12th ed.): Whitehouse Station, N.J., Merck and Company, Inc. [variously paged].

California Environmental Protection Agency, 1999, Final prioritized candidate chemicals under consideration for carcinogenicity evaluation—fifty-four chemicals within batch #3, accessed July 30, 2010, at *http://www.oehha.ca.gov/prop65/pdf/fbatch3.pdf*.

CambridgeSoft Corporation, 2010, Chembiofinder.com database, accessed July 30, 2010, at *http://www.cambridgesoft.com/*.

Carter, J.M., Delzer, G.C., Kingsbury, J.A., and Hopple, J.A., 2007, Concentration data for anthropogenic organic compounds in groundwater, surface water, and finished water of selected community water systems in the United States, 2002–05: U.S. Geological Survey Data Series 268, 30 p., accessed August 3, 2010, at *http://pubs.usgs.gov/ds/2007/268/*.

Chemicalland21, 2010, Tolutraizole, accessed July 30, 2010, at *http://www.chemicalland21.com/specialtychem/finechem/TOLUTRIAZOLE.htm*.

Childress, C.J.O., Foreman, W.T., Connor, B.F., and Maloney, T.J., 1999, New reporting procedures based on long-term method detection levels and some considerations for interpretations of water-quality data provided by the U.S. Geological Survey National Water Quality Laboratory: U.S. Geological Survey Open-File Report 99–193, 19 p.

Cohen, D.B., Gilmore, D., Fischer, C., and Bowes, G., 1983, Water quality and pesticides—1,2–Dichloropropane (1,2–D) and 1,3–dichloropropene (1,3–D): Sacramento, Calif., California State Water Resources Control Board, Water Quality and Pesticides Special Projects Report No. 83–8SP.

Connor, B.F., Rose, D.L., Noriega, M.C., Murtagh, L.K., and Abney, S.R., 1998, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—Determination of 86 volatile organic compounds in water by gas chromatography/mass spectrometry, including detections less than reporting limits: U.S. Geological Survey Open-File Report 97–829, 78 p.

Cozzarelli, I.M., Baedecker, M.J., Eganhouse, R.P., and Goerlitz, D.F., 1994, The geochemical evolution of low-molecular-weight organic acids derived from the degradation of petroleum contaminants in groundwater: Geochimica et Cosmochimica Acta, v. 58, no. 2, p. 863–877.

Cozzarelli, I.M., Eganhouse, R.P., and Baedecker, M.J., 1990, Transformation of monoaromatic hydrocarbons to organic acids in anoxic groundwater environment: Environmental Geology, v. 16, no. 2, p. 135–141.

Delzer, G.C., and Hamilton, P.A., 2007, National Water-Quality Assessment Program—Source Water-Quality Assessments: U.S. Geological Survey Fact Sheet 2007–3069, 2 p. (Also available at *http://pubs.usgs.gov/fs/2007/3069/*.)

Egli, Christine; Tschan, Thomas; Scholtz, Rudolf; Cook, A.M.; and Leisinger, Thomas, 1988, Transformation of tetrachloromethane to dichloromethane and carbon dioxide by acetobacterium woodii: Applied and Environmental Microbiology, v. 54, no. 11, p. 2,819–2,824.

Furlong, E.T., Anderson, B.D., Werner, S.L., Soliven, P.P., Coffey, L.J., and Burkhardt, M.R., 2001, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—Determination of pesticides in water by graphitized carbon-based solid-phase extraction and high-performance liquid chromatography/mass spectrometry: U.S. Geological Survey Water-Resources Investigations Report 01–4134, 73 p.

Gilliom, R.J., Alley, W.M., and Gurtz, M.E., 1995, Design of the National Water-Quality Assessment Program—Occurrence and distribution of water-quality conditions: U.S. Geological Survey Circular 1112, 33 p.

Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Cahill, J.D., Zaugg, S.D., Werner, S.L., Meyer, M.T., Kryak, D.D., 2005, Transport of chemical and microbial compounds from known wastewater discharges—Potential for use as indicators of human fecal contamination: Environmental Science and Technology, v. 39, p. 5,157–5,169.

Haag, W.R., and Mill, T., 1988, Effect of a subsurface sediment on hydrolysis of haloalkanes and epoxides: Environmental Science and Technology, v. 22, no. 6, p. 658–663.

Hladik, M.L., Hsiao, J.J., and Roberts, A.L., 2005, Are neutral chloroacetamide herbicide degradates of potential environmental concern? Analysis and occurrence in the Upper Chesapeake Bay: Environmental Science and Technology, v. 39, no. 17, p. 6,561–6,574.

Hopple, J.A., Delzer, G.C., and Kingsbury, J.A., 2009, Anthropogenic organic compounds in source water of selected community water systems that use groundwater, 2002–05: U.S. Geological Survey Scientific Investigations Report 2009–5200, 74 p. (Also available at *http://pubs.usgs.gov/sir/2009/5200/*.)

Kingsbury, J.A., Delzer, G.C., and Hamilton, P.A., 2008a, Man-made organic compounds in source water of nine community water systems that withdraw from streams, 2002–05: U.S. Geological Survey Fact Sheet 2008–3094, 6 p. (Also available at *http://pubs.usgs.gov/fs/2008/3094/*.)

Kingsbury, J.A., Delzer, G.C., and Hopple, J.A., 2008b, Anthropogenic organic compounds in source water of nine community water systems that withdraw from streams, 2002–05: U.S. Geological Survey Scientific Investigations Report 2008–5208, 66 p. (Also available at *http://pubs.usgs.gov/sir/2008/5208/*.)

Klecka, G.M., Gonsoir, S.J., and Markham, D.A., 1990, Biological transformations of 1,1,1-trichloroethane in subsurface soils and groundwater: Environmental Toxicology and Chemistry, v. 9, no. 12, p. 1,437–1,451.

Kolpin, D.W., Furlong, E.T., Meyer, M.T., Thurman, E.M., Zaugg, S.D., Barber, L.B., and Buxton, H.T., 2002, Pharmaceuticals, hormones, and other organic wastewater contaminants in U.S. streams, 1999-2000—A national reconnaissance: Environmental Science and Technology, v. 36, no. 6, p. 1,202–1,211.

Koterba, M.T., Wilde, F.D., and Lapham, W.W., 1995, Groundwater data-collection protocols and procedures for the National Water-Quality Assessment Program—Collection and documentation of water-quality samples and related data: U.S. Geological Survey Open-File Report 95–399, 113 p.

Lee, E.A., and Strahan, A.P., 2003, Methods of analysis by the U.S. Geological Survey Organic Geochemistry Research Group—Determination of acetamide herbicides and their degradation products in water using online solid-phase extraction and liquid chromatography/mass spectrometry: U.S. Geological Survey Open-File Report 03–173, 17 p.

Lindley, C.E., Stewart, J.T., and Sandstrom, M.W., 1996, Determination of low concentrations of acetochlor in water by automated solid-phase extraction and gas chromatography with mass selective detection: Journal of Association of Official Analytical Chemists International, v. 79, no. 4, p. 962–966.

Lorah, M.M., and Olsen, L.D., 1999, Natural attenuation of chlorinated volatile organic compounds in a freshwater tidal wetland—Field evidence of anaerobic biodegradation: Water Resources Research, v. 35, no. 12, p. 3,811–3,828.

Madsen, J.F., Sandstrom, M.W., and Zaugg, S.D., 2003, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—A method supplement for the determination of fipronil and degradates in water by gas chromatography/mass spectrometry: U.S. Geological Survey Open-File Report 02–462, 11 p.

Martin, J.D., 2002, Variability of pesticide detections and concentrations in field replicate water samples collected for the National Water-Quality Assessment Program, 1992–97: U.S. Geological Survey Water-Resources Investigations Report 01–4178, 84 p.

Megonigal, J.P., Hines, M.E., and Visscher, P.T., 2004, Anaerobic metabolism—Linkages to trace gases and aerobic processes, in Schlesinger, W.H., ed., Biogeochemistry: Oxford, United Kingdom, Elsevier-Pergamon, p. 317–424, accessed July 30, 2010, at *http://serc.si.edu/labs/biogeochem/publications/Megonigal_Hines_Visscher_2004_V2.pdf*.

Munch, J.W., 1995, Method 524.2.—Measurement of purgeable organic compounds in water by capillary column gas chromatography/mass spectrometry, revision 4.1: Cincinnati, Ohio, Environmental Monitoring Systems Laboratory, U.S. Environmental Protection Agency, 48 p.

National Oceanic and Atmospheric Administration, 2008, Air Resources Laboratory, accessed July 30, 2010, at *http://www.arl.noaa.gov/faq/ac4.html*.

Pankow, J.F., Rathbun, R.E., and Zogorski, J.S., 1996, Calculated volatilization rates of fuel oxygenate compounds and other gasoline-related compounds from rivers and streams: Chemosphere, v. 33, no. 5, p. 921–937.

Rose, D.L., and Sandstrom, M.W., 2003, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—Determination of gasoline oxygenates, selected degradates, and BTEX in water by heated purge and trap/gas chromatography/mass spectrometry: U.S. Geological Survey Water-Resources Investigations Report 03–4079, 31 p.

Sandstrom, M.W., Stroppel, M.E., Foreman, W.T., and Schroeder, M.P., 2001, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—Determination of moderate-use pesticides and selected degradates in water by C–18 solid-phase extraction and gas chromatography/mass spectrometry: U.S. Geological Survey Water-Resources Investigations Report 01–4098, 70 p.

Scorecard, 2006, Chemical profiles, accessed December 22, 2006, at *http://www.scorecard.org/chemical-profiles/index.tcl*.

Spectrum Laboratories Inc., 2010a, Chemical fact sheet, accessed July 30, 2010, at *http://www.speclab.com/compound/c80626.htm*.

Spectrum Laboratories Inc., 2010b, Chemical fact sheet, accessed July 30, 2010, at *http://www.speclab.com/compound/c591786.htm*.

Tesoriero, A.J., Loffler, F.E., and Liebscher, Hugh, 2001, Fate and origin of 1,2-dichloropropane in an unconfined shallow aquifer: Environmental Science and Technology, v. 35, no. 3, p. 455–461.

Toccalino, P.L., Norman, J.E., and Hitt, K.J., 2010, Quality of source water from public-supply wells in the United States, 1993–2007: U.S. Geological Survey Scientific Investigations Report 2010–5024, 209 p. (Also available at *http://pubs.usgs.gov/sir/2010/5024/*.)

United Nations Environmental Programme, 2002, Methyl acrylonitrile, accessed July 30, 2010, at *http://www.chem.unep.ch/irptc/sids/OECDSIDS/126987.pdf*.

U.S. Environmental Protection Agency, 2006, Iodomethane risk assessment; notice of availability, accessed July 30, 2010, at *http://www.epa.gov/fedrgstr/EPA-PEST/2006/January/Day-06/p28.htm*.

U.S. Environmental Protection Agency, 2009, Inert (other) pesticide ingredients in pesticide products—Categorized list of inert (other) pesticide ingredients, accessed July 29, 2010, at *http://www.epa.gov/opprd001/inerts/lists.html*.

U.S. Environmental Protection Agency, 2010, Public drinking water systems—Facts and figures, accessed July 29, 2010, at *http://www.epa.gov/safewater/pws/factoids.html*.

U.S. Geological Survey, variously dated, National field manual for the collection of water-quality data: U.S. Geological Survey Techniques of Water-Resources Investigations, book 9, chaps. A1–A9, accessed July 29, 2010, at *http://pubs.water.usgs.gov/twri9A*.

U.S. Geological Survey, 2003, Principal aquifers of the 48 conterminous United States, Hawaii, Puerto Rico, and the U.S. Virgin Islands, accessed March 1, 2007, at *http://www.nationalatlas.gov/mld/aquifrp.html*.

U.S. Geological Survey, 2007, Toxic Substances Hydrology Program—Fuel oxygenates, accessed January 17, 2007, at *http://toxics.usgs.gov/definitions/fuel_oxygenates.html*.

U.S. National Library of Medicine, 2010, Household products database, accessed July 30, 2010, at *http://householdproducts.nlm.nih.gov/*.

U.S. National Library of Medicine, 2006, TOXNET—Toxicology data network, accessed December 22, 2006, at *http://toxnet.nlm.nih.gov/*.

Valder, J.F., Delzer, G.C., Price, C.V., and Sandstrom, M.W., 2008, Study design and percent recoveries of anthropogenic organic compounds with and without the addition of ascorbic acid to preserve water samples containing free chlorine, 2004–06: U.S. Geological Survey Open-File Report 2008–1226, 85 p., accessed October 6, 2010, at *http://pubs.usgs.gov/of/2008/1226/*.

Vogel, T.M., and McCarty, P.L., 1985, Biotransformation of tetrachloroethylene to trichloroethylene, dichloroethylene, vinyl chloride, and carbon dioxide under methanogenic conditions: Applied and Environmental Microbiology, v. 49, no. 5, p. 1,080–1,083.

Wiedemeier, T.H., Swanson, M.A., Wilson, J.T., Kampbell, D.H., Miller, R.H., and Hansen, J.E., 1996, Approximation of biodegradation rate constants for monoaromatic hydrocarbons (BTEX) in groundwater: Groundwater Monitoring and Remediation, v.16, no. 3, p. 186–194.

Wood, Alan, 2010, Compendium of pesticide common names, accessed July 29, 2010, at *http://www.alanwood.net/pesticides/index_cn_frame.html*.

Zaugg, S.D., Sandstrom, M.W., Smith, S.G., and Fehlberg, K.M., 1995, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—Determination of pesticides in water by C–18 solid-phase extraction and capillary-column gas chromatography/mass spectrometry with selected-ion monitoring: U.S. Geological Survey Open-File Report 95–181, 49 p.

Zaugg, S.D., Smith, S.G., Schroeder, M.P., Barber, L.B., and Burkhardt, M.R., 2002, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory—Determination of wastewater compounds by polystyrene-divinylbenzene solid-phase extraction and capillary-column gas chromatography/mass spectrometry: U.S. Geological Survey Water-Resources Investigations Report 01–4186, 37 p.

Zogorski, J.S., Carter, J.M., Ivahnenko, Tamara, Lapham, W.W., Moran, M.J., Rowe, B.L., Squillace, P.J., and Toccalino, P.L, 2006, The quality of our Nation's waters—Volatile organic compounds in the Nation's groundwater and drinking-water supply wells: U.S. Geological Survey Circular 1292, 101 p.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
				Disinfection by-products	
SH2020	Bromodichloromethane	32101	75–27–4	Trihalomethane, organic synthesis, fire extinguishers	Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2020	Bromoform	32104	75–25–2	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.
SH2020	Chloroform	32106	67–66–3	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.
SH2020	Dibromochloromethane	32105	124–48–1	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	
SH2020	1,2-Dibromo-3-chloropropane (DBCP)	82625	96–12–8	Organic synthesis, nematocide	Budavari, 1989; Zogorski and others, 2006.
SH2020	1,2-Dibromoethane (EDB)	77651	106–93–4	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.
SH2020	1,2-Dichloropropane	34541	78–87–5	Dry-cleaning solvent, chemical intermediate, stain remover	Budavari, 1989, 1996; Tesoriero and others, 2001; Zogorski and others, 2006.
SH2020	1,3-Dichloropropane	77173	142–28–9	Fumigant contaminant	Bender and others, 1999.
SH2020	1,4-Dichlorobenzene (*p*-dichlorobenzene)	34571	106–46–7	Deodorizer, moth killer, manufacture of dyes, chemical intermediate	Bender and others, 1999; Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006.
SH2020	2,2-Dichloropropane	77170	594–20–7	Fumigant contaminant	Cohen and others, 1983; Bender and others, 1999.
SH2020	Bromomethane (methyl bromide)	34413	74–83–9	Solvent, chemical intermediate	Bender and others, 1999; Zogorski and others, 2006.
SH2020	*cis*-1,3-Dichloropropene	34704	10061–01–5	Solvent, chemical intermediate	Bender and others, 1999; Zogorski and others, 2006.
SH2020	*trans*-1,3-Dichloropropene	34699	10061–02–6	Solvent, chemical intermediate	Bender and others, 1999; Zogorski and others, 2006.
				Fungicides and fungicide degradates	
SH2033	3,5-Dichloroaniline	61627	626–43–7	--	Sandstrom and others, 2001.
SH2060	Benomyl	50300	17804–35–2	--	Furlong and others, 2001; Wood, 2010.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Fungicides and fungicide degradates—Continued		
SH2060	Chlorothalonil	49306	1897–45–6	--	Furlong and others, 2001.
SH2033	*cis*-Propiconazole	79846	c–60207–90–1[b]	--	Sandstrom and others, 2001.
SH2003/2033	Iprodione	61593	36734–19–7	--	Sandstrom and others, 2001; Wood, 2010.
SH2003/2033	Metalaxyl	61596	57837–19–1	--	Furlong and others, 2001; Glassmeyer and others, 2005; Wood, 2010.
SH2003/2033	Myclobutanil	61599	88671–89–0	--	Sandstrom and others, 2001: Wood, 2010.
SH1433	Pentachlorophenol	34459	87–86–5	Wood preservative, herbicide, insecticide, plant growth regulator	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; Wood, 2010.
SH2060	Propiconazole	50471	60207–90–1	--	Furlong and others, 2001; Wood, 2010.
SH2033	Tebuconazole	62852	107534–96–3	--	Wood, 2010.
SH2033	*trans*-Propiconazole	79847	t–60207–90–1[b]	--	Sandstrom and others, 2001.
			Gasoline hydrocarbons, oxygenates, and oxygenate degradates		
SH2020	1,2,3,4-Tetramethylbenzene	49999	488–23–3	Petroleum hydrocarbon	Cozzarelli and others, 1994.
SH2020	1,2,3,5-Tetramethylbenzene	50000	527–53–7	Petroleum hydrocarbon	Cozzarelli and others, 1990.
SH2020	1,2,3-Trimethylbenzene	77221	526–73–8	Gasoline hydrocarbon, pesticide adjuvant	Wiedemeier and others, 1996; U.S. Environmental Protection Agency, 2009.
SH2020	1,2,4-Trimethylbenzene	77222	95–63–6	Petroleum hydrocarbon, pesticide adjuvant, chemical intermediate	Cozzarelli and others, 1990; Wiedemeier and others, 1996; U.S. Environmental Protection Agency, 2009; U.S. National Library of Medicine, 2006.
SH2020	1,3,5–Trimethylbenzene	77226	108–67–8	Used in synthesis of Ethanox 330, gasoline hydrocarbon	Wiedemeier and others, 1996; U.S. National Library of Medicine, 2006.
SH2020	1-Ethyl-2-methylbenzene	77220	611–14–3	Petroleum hydrocarbon	Cozzarelli and others, 1990; Zogorski and others, 2006.
SH1433	1-Methylnaphthalene	62054	90–12–0	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, 2009.
SH1433	2,6-Dimethylnaphthalene	62055	581–42–0	Polynuclear aromatic hydrocarbon, diesel fuel component, pesticide adjuvant, insecticide	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH1433	2-Methylnaphthalene	62056	91–57–6	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, 2009.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Gasoline hydrocarbons, oxygenates, and oxygenate degradates—Continued		
SH2020	Benzene	34030	71–43–2	Gasoline hydrocarbon, organic synthesis	Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2020	Diisopropyl ether (DIPE)	81577	108–20–3	Gasoline oxygenate, solvent	Bender and others, 1999.
SH2020	Ethyl *tert*-butyl ether (ETBE)	50004	637–92–3	Gasoline oxygenate	Bender and others, 1999.
SH2020	Ethylbenzene	34371	100–41–4	Gasoline hydrocarbon, organic synthesis, solvent, pesticide adjuvant	Bender and others, 1999; U.S. National Library of Medicine, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	Isopropylbenzene	77223	98–82–8	Organic synthesis, building materials, solvent, gasoline hydrocarbon, intermediate in production of plastics	Bender and others, 1999; Glassmeyer and others, 2005.
SH2020	*m*- & *p*-Xylene	85795	106–42–3; 108–38–3	Gasoline hydrocarbon, solvent, organic synthesis	U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
SH2020	Methyl *tert*-butyl ether (MTBE)	78032	1634–04–4	Gasoline oxygenate	Bender and others, 1999.
SH2020	Naphthalene	34696	91–20–3	Polynuclear aromatic hydrocarbon, petroleum hydrocarbon, pesticide adjuvant, combustion product, disinfectant, antiseptic, mouthwash, throat lozenges, slimicides, manufacture of synthetic fibers, fumigant, moth repellant	Bender and others, 1999; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
SH2020	*n*-Butylbenzene	77342	104–51–8	Solvent, organic synthesis	Bender and others, 1999; U.S. National Library of Medicine, 2006; Zogorski and others, 2006.
SH2020	*o*-Xylene	77135	95–47–6	Gasoline hydrocarbon, pesticide adjuvant, organic synthesis, solvent	Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2020	*p*-Isopropyltoluene (*p*-cymene)	77356	99–87–6	Organic synthesis, solvent, heat transfer agent, wood office furniture	Bender and others, 1999; Scorecard, 2006; U.S. National Library of Medicine, 2006.
SH2020	*sec*-Butylbenzene	77350	135–98–8	Gasoline hydrocarbon, solvent, organic synthesis, plasticizer	Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2020	Styrene	77128	100–42–5	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.
SH4024	*tert*-Amyl alcohol (2-methyl-2-butanol)	77073	75–85–4	Gasoline oxygenate	U.S. Geological Survey, 2007.
SH2020	*tert*-Amyl methyl ether (TAME)	50005	994–05–8	Gasoline oxygenate	Bender and others, 1999.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Gasoline hydrocarbons, oxygenates, and oxygenate degradates—Continued		
SH4024	*tert*-Butyl alcohol	77035	75–65–0	Gasoline oxygenate; methyl tert-butyl ether (MTBE) degradate	Pankow and others, 1996; Bradley and others, 2001; U.S. Geological Survey, 2007.
SH2020	*tert*-Butylbenzene	77353	98–06–6	Organic synthesis	Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2020	Toluene	34010	108–88–3	Solvent consumer products, pesticide adjuvant	Bender and others, 1999; U.S. Environmental Protection Agency, 2009.
			Herbicides and herbicide degradates		
SH2060	2,4–D	39732	94–75–7	--	Furlong and others, 2001.
SH2060	2,4–D methyl ester	50470	1928–38–7	--	Furlong and others, 2001.
SH2060	2,4–DB	38746	94–82–6	--	Furlong and others, 2001.
SH2003/2033	2,6-Diethylaniline	82660	579–66–8	Herbicide (mostly alachlor) degradate	Zaugg and others, 1995; Hladik and others, 2005.
SH2003/2033	2-Chloro-2,6-diethyl-acetanilide	61618	6967–29–9	Herbicide (mostly alachlor) degradate	Sandstrom and others, 2001; Hladik and others, 2005.
SH2003/2033	2-Ethyl-6-methyl-aniline	61620	24549–06–2	Herbicide (acetochlor or metolachlor) degradate	Sandstrom and others, 2001; Hladik and others, 2005.
SH2060	2-Hydroxyatrazine	50355	2163–68–0	Herbicide (atrazine) degradate	Furlong and others, 2001.
SH2060	3(4-Chlorophenyl)-1-methyl urea	61692	5352–88–5	Herbicide degradate	Furlong and others, 2001.
SH2003/2033	3,4-Dichloroaniline	61625	95–76–1	Herbicide (diuron) degradate	Sandstrom and others, 2001.
SH2003/2033	4-Chloro-2-methyl-phenol	61633	1570–64–5	Herbicide (MCPA) degradate	Sandstrom and others, 2001.
SH2003/2033	Acetochlor	49260	34256–82–1	--	Lee and Strahan, 2003.
LCPD	Acetochlor ethane sulfonic acid	61029	187022–11–3	Herbicide (acetochlor) degradate	Lee and Strahan, 2003.
LCPD	Acetochlor oxanilic acid	61030	184992–44–4	Herbicide (acetochlor) degradate	Lee and Strahan, 2003.
LCPD	Acetochlor sulfynil-acetic acid	62847	--	Herbicide (acetochlor) degradate	Lee and Strahan, 2003.
LCPD	Acetochlor/meto-lachlor ethane sulfonic acid 2nd amide	62850	--	Herbicide (acetochlor or metolachlor) degradate	Lee and Strahan, 2003.
SH2060	Acifluorfen	49315	50594–66–6	--	Furlong and others, 2001.
SH2003/2033	Alachlor	46342	15972–60–8	--	Zaugg and others, 1995.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Herbicides and herbicide degradates—Continued		
LCPD	Alachlor ethane sulfonic acid	50009	142363–53–9	Herbicide (alachlor) degradate	Lee and Strahan, 2003.
LCPD	Alachlor ethane sulfonic acid 2nd amide	62849	--	Herbicide (alachlor) degradate	Lee and Strahan, 2003.
LCPD	Alachlor oxanilic acid	61031	171262–17–2	Herbicide (alachlor) degradate	Lee and Strahan, 2003.
LCPD	Alachlor sulfynilacetic acid	62848	140939–16–8	Herbicide (alachlor) degradate	Lee and Strahan, 2003.
SH2003/2033	Atrazine	39632	1912–24–9	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
SH2003/2033	Benfluralin	82673	1861–40–1	--	Zaugg and others, 1995.
SH2060	Bensulfuron-methyl	61693	83055–99–6	--	Furlong and others, 2001.
SH2060	Bentazon	38711	25057–89–0	--	Furlong and others, 2001.
SH2060	Bromacil	04029	314–40–9	--	Furlong and others, 2001; Glassmeyer and others, 2005.
SH2060	Bromoxynil	49311	1689–84–5	--	Furlong and others, 2001.
SH2060	Chloramben, methyl ester	61188	7286–84–2	--	Furlong and others, 2001.
SH2060	Chlorimuron-ethyl	50306	90982–32–4	--	Furlong and others, 2001.
SH2060	Clopyralid	49305	1702–17–6	--	Furlong and others, 2001.
SH2033	Cyanazine	04041	21725–46–2	--	Zaugg and others, 1995.
SH2060	Cycloate	04031	1134–23–2	--	Furlong and others, 2001.
SH2003/2033	Dacthal	82682	1861–32–1	--	Zaugg and others, 1995.
SH2060	Dacthal monoacid	49304	887–54–7	Herbicide (dacthal) degradate	Furlong and others, 2001.
SH2003/2033	Deethylatrazine	04040	6190–65–4	Herbicide (atrazine) degradate	Zaugg and others, 1995.
SH2060	Deethyldeisopropyl-atrazine	04039	3397–62–4	Herbicide (atrazine) degradate	Furlong and others, 2001.
SH2060	Deisopropylatrazine	04038	1007–28–9	Herbicide (atrazine) degradate	Furlong and others, 2001.
SH2060	Dicamba	38442	1918–00–9	--	Furlong and others, 2001.
SH2060	Dichlorprop	49302	120–36–5	--	Furlong and others, 2001.
LCPD	Dimethenamid	61588	87674–68–8	--	Lee and Strahan, 2003.
LCPD	Dimethenamid ethane sulfonic acid	61951	205939–58–8	Herbicide (dimethenamid) degradate	Lee and Strahan, 2003.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Herbicides and herbicide degradates—Continued		
LCPD	Dimethenamid oxanilic acid	62482	--	Herbicide (dimethenamid) degradate	Lee and Strahan, 2003.
SH2060	Dinoseb	49301	88–85–7	Plant growth regulator	Furlong and others, 2001.
SH2060	Diphenamid	04033	957–51–7	--	Furlong and others, 2001.
SH2060	Diuron	49300	330–54–1	--	Furlong and others, 2001.
SH2033	EPTC	82668	759–94–4	--	Zaugg and others, 1995; Wood, 2010.
SH2060	Fenuron	49297	101–42–8	--	Furlong and others, 2001.
LCPD	Flufenacet	62481	142459–58–3	--	Lee and Strahan, 2003.
LCPD	Flufenacet ethane sulfonic acid	61952	--	Herbicide (flufenacet) degradate	Lee and Strahan, 2003.
LCPD	Flufenacet oxanilic acid	62483	--	Herbicide (flufenacet) degradate	Lee and Strahan, 2003.
SH2060	Flumetsulam	61694	98967–40–9	--	Furlong and others, 2001.
SH2060	Fluometuron	38811	2164–17–2	--	Furlong and others, 2001.
SH2003/2033	Hexazinone	04025	51235–04–2	--	Sandstrom and others, 2001.
SH2060	Imazaquin	50356	81335–37–7	--	Furlong and others, 2001.
SH2060	Imazethapyr	50407	81335–77–5	--	Furlong and others, 2001.
SH2060	Linuron	38478	330–55–2	--	Furlong and others, 2001.
SH2060	MCPA	38482	94–74–6	--	Furlong and others, 2001.
SH2060	MCPB	38487	94–81–5	--	Furlong and others, 2001.
SH2003/2033	Metolachlor	39415	51218–45–2	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
LCPD	Metolachlor ethane sulfonic acid	61043	171118–09–5	Herbicide (metolachlor) degradate	Lee and Strahan, 2003.
LCPD	Metolachlor oxanilic acid	61044	152019–73–3	Herbicide (metolachlor) degradate	Lee and Strahan, 2003.
SH2003/2033	Metribuzin	82630	21087–64–9	--	Zaugg and others, 1995.
SH2060	Metsulfuron methyl	61697	74223–64–6	--	Furlong and others, 2001.
SH2033	Molinate	82671	2212–67–1	--	Zaugg and others, 1995.
SH2060	Neburon	49294	555–37–3	--	Furlong and others, 2001.
SH2060	Nicosulfuron	50364	111991–09–4	--	Furlong and others, 2001.
SH2060	Norflurazon	49293	27314–13–2	--	Furlong and others, 2001.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Herbicides and herbicide degradates—Continued		
SH2060	Oryzalin	49292	19044–88–3	--	Furlong and others, 2001.
SH2033	Oxyfluorfen	61600	42874–03–3	--	Sandstrom and others, 2001.
SH2003/2033	Pendimethalin	82683	40487–42–1	--	Zaugg and others, 1995.
SH2060	Picloram	49291	1918–02–1	--	Furlong and others, 2001.
SH2003/2033	Prometon	04037	1610–18–0	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
SH2003/2033	Prometryn	04036	7287–19–6	--	Sandstrom and others, 2001.
LCPD	Propachlor	04024	1918–16–7	--	Lee and Strahan, 2003.
LCPD	Propachlor ethane sulfonic acid	62766	--	Herbicide (propachlor) degradate	Lee and Strahan, 2003.
LCPD	Propachlor oxanilic acid	62767	--	Herbicide (propachlor) degradate	Lee and Strahan, 2003.
SH2033	Propanil	82679	709–98–8	--	Zaugg and others, 1995.
SH2060	Propham	49236	122–42–9	--	Furlong and others, 2001.
SH2003/2033	Propyzamide	82676	23950–58–5	--	Zaugg and others, 1995.
SH2060	Siduron	38548	1982–49–6	--	Furlong and others, 2001.
SH2003/2033	Simazine	04035	122–34–9	--	Zaugg and others, 1995.
SH2060	Sulfometuron-methyl	50337	74222–97–2	--	Furlong and others, 2001.
SH2060/2033	Tebuthiuron	82670	34014–18–1	--	Furlong and others, 2001.
SH2060	Terbacil	04032	5902–51–2	--	Furlong and others, 2001.
SH2003/2033	Terbuthylazine	04022	5915–41–3	--	Sandstrom and others, 2001.
SH2033	Thiobencarb	82681	28249–77–6	--	Zaugg and others, 1995.
SH2060	Triclopyr	49235	55335–06–3	--	Furlong and others, 2001.
SH2003/2033	Trifluralin	82661	1582–09–8	--	Zaugg and others, 1995.
			Insecticides and insecticide degradates		
SH2003/2033	1-Naphthol	49295	90–15–3	Herbicide (napropamide) and insecticide (carbaryl) degradate	Sandstrom and others, 2001.
SH2060	3-Hydroxycarbofuran	49308	16655–82–6	Insecticide (carbofuran) degradate	Furlong and others, 2001.
SH2060	3-Ketocarbofuran	50295	16709–30–1	Insecticide (carbofuran) degradate	Furlong and others, 2001.
SH2060	Aldicarb	49312	116–06–3	--	Furlong and others, 2001.
SH2060	Aldicarb sulfone	49313	1646–88–4	Insecticide (aldicarb) degradate	Furlong and others, 2001.
SH2060	Aldicarb sulfoxide	49314	1646–87–3	Insecticide (aldicarb) degradate	Furlong and others, 2001.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Insecticides and insecticide degradates—Continued		
SH2033	*alpha*-Endosulfan	34362	959–98–8	--	Sandstrom and others, 2001.
SH2003/2033	Azinphos-methyl	82686	86–50–0	--	Zaugg and others, 1995.
SH2003/2033	Azinphos-methyl-oxon	61635	961–22–8	Insecticide (azinphos-methyl) degradate	Sandstrom and others, 2001.
SH2060	Bendiocarb	50299	22781–23–3	--	Furlong and others, 2001.
SH2060/2033	Carbaryl	49310/82680	63–25–2	--	Furlong and others, 2001; Glassmeyer and others, 2005.
SH2060/2033	Carbofuran	49309/82674	1563–66–2	--	Furlong and others, 2001; Zaugg and others, 1995.
SH2003/2033	Chlorpyrifos	38933	2921–88–2	--	Zaugg and others, 1995; Glassmeyer and others, 2005.
SH2003/2033	Chlorpyrifos, oxygen analog	61636	5598–15–2	Insecticide (chlorpyrifos) degradate	Sandstrom and others, 2001.
SH2003/2033	*cis*-Permethrin	82687	54774–45–7	--	Zaugg and others, 1995.
SH2003/2033	Cyfluthrin	61585	68359–37–5	--	Sandstrom and others, 2001.
SH2003/2033	Cypermethrin	61586	52315–07–8	--	Sandstrom and others, 2001.
SH2003/2033	Desulfinylfipronil	62170	--	Insecticide (fipronil) degradate	Madsen and others, 2003.
SH2003/2033	Desulfinylfipronil amide	62169	--	Insecticide (fipronil) degradate	Madsen and others, 2003.
SH2003/2033	Diazinon	39572	333–41–5	--	Zaugg and others, 1995; Sandstrom and others, 2001; Glassmeyer and others, 2005.
SH2003/2033	Diazinon, oxygen analog	61638	962–58–3	Insecticide (diazinon) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2003/2033	Dichlorvos	38775	62–73–7	--	Zaugg and others, 1995; Sandstrom and others, 2001; Glassmeyer and others, 2005.
SH2003/2033	Dicrotophos	38454	141–66–2	--	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2003/2033	Dieldrin	39381	60–57–1	--	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2003/2033	Dimethoate	82662	60–51–5	--	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2033	Disulfoton	82677	298–04–4	--	Zaugg and others, 1995.
SH2033	Disulfoton sulfone	61640	2497–06–5	Insecticide (disulfoton) degradate	Sandstrom and others, 2001.
SH2033	Endosulfan sulfate	61590	1031–07–8	Insecticide (alpha-endosulfan) degradate	Sandstrom and others, 2001.
SH2003/2033	Ethion	82346	563–12–2	--	Zaugg and others, 1995; Sandstrom and others, 2001.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Insecticides and insecticide degradates—Continued		
SH2003/2033	Ethion monoxon	61644	17356–42–2	Insecticide (ethion) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2033	Ethoprophos	82672	13194–48–4	--	Zaugg and others, 1995.
SH2003/2033	Fenamiphos	61591	22224–92–6	--	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2003/2033	Fenamiphos sulfone	61645	31972–44–8	Insecticide (fenamiphos) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2003/2033	Fenamiphos sulfoxide	61646	31972–43–7	Insecticide (fenamiphos) degradate	Zaugg and others, 1995; Sandstrom and others, 2001.
SH2003/2033	Fipronil	62166	120068–37–3	--	Madsen and others, 2003.
SH2003/2033	Fipronil sulfide	62167	120067–83–6	Insecticide (fipronil) degradate	Madsen and others, 2003.
SH2003/2033	Fipronil sulfone	62168	120068–36–2	Insecticide (fipronil) degradate	Madsen and others, 2003.
SH2003/2033	Fonofos	04095	944–22–9	--	Zaugg and others, 1995.
SH2003	Fonofos, oxygen analog	61649	944–21–8	Insecticide (fonofos) degradate	Sandstrom and others, 2001.
SH2060	Imidacloprid	61695	138261–41–3	--	Furlong and others, 2001.
SH2003/2033	Isofenphos	61594	25311–71–1	--	Sandstrom and others, 2001.
SH2033	*lambda*-Cyhalothrin	61595	91465–08–6	--	Wood, 2010.
SH2003/2033	Malaoxon	61652	1634–78–2	Insecticide (malathion) degradate	Sandstrom and others, 2001.
SH2003/2033	Malathion	39532	121–75–5	--	Zaugg and others, 1995.
SH2003/2033	Methidathion	61598	950–37–8	--	Sandstrom and others, 2001.
SH2060	Methiocarb	38501	2032–65–7	--	Furlong and others, 2001.
SH2060	Methomyl	49296	16752–77–5	--	Furlong and others, 2001.
SH2060	Oxamyl	38866	23135–22–0	--	Furlong and others, 2001.
SH2003/2033	Paraoxon-methyl	61664	950–35–6	Insecticide (methyl parathion) degradate	Sandstrom and others, 2001.
SH2003/2033	Parathion-methyl	82667	298–00–0	--	Zaugg and others, 1995.
SH2003/2033	Phorate	82664	298–02–2	--	Zaugg and others, 1995.
SH2003/2033	Phorate oxon	61666	2600–69–3	Insecticide (phorate) degradate	Sandstrom and others, 2001.
SH2003/2033	Phosmet	61601	732–11–6	--	Sandstrom and others, 2001.
SH2003/2033	Phosmet oxon	61668	3735–33–9	Insecticide (phosmet) degradate	Sandstrom and others, 2001.
SH2033	Propargite	82685	2312–35–8	--	Zaugg and others, 1995.
SH2060	Propoxur	38538	114–26–1	--	Furlong and others, 2001.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
				Insecticides and insecticide degradates—Continued	
SH2033	Tefluthrin	61606	79538–32–2	--	Sandstrom and others, 2001.
SH2003/2033	Terbufos	82675	13071–79–9	--	Zaugg and others, 1995.
SH2003/2033	Terbufos oxygen analogue sulfone	61674	56070–15–6	Insecticide (terbufos) degradate	Sandstrom and others, 2001.
				Manufacturing additives	
SH1433	5-Methyl-1H-benzotriazole	62063	136–85–6	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; Chemicalland21, 2010.
SH1433	Bisphenol A	62069	80–05–7	Used in manufacture of plastic and polycarbonate resins	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
SH1433	Tri(2-butoxyethyl) phosphate	62093	78–51–3	Plasticizer, pesticide adjuvant, flame retardant	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. Environmental Protection Agency, 2009.
SH1433	Tri(2-chloroethyl) phosphate	62087	115–96–8	Flame retardant, fire resistant cellulose plasticizer	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Tributyl phosphate	62089	126–73–8	Antifoaming agent and flame retardant	Zaugg and others, 2002.
SH1433	Triphenyl phosphate	62092	115–86–6	Plasticizer, flame retardant	Budavari, 1989; Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Tris(dichlorisopropyl) phosphate	62088	13674–87–8	Flame retardant, plasticizer	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
				Organic synthesis compounds	
SH2020	1,1-Dichloropropene	77168	563–58–6	Solvent (pharmaceuticals)	Bender and others, 1999; Scorecard, 2006.
SH2020	1,2,3-Trichlorobenzene	77613	87–61–6	Termiticide, solvent	Budavari, 1989, 1996; Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2020	1,2,3-Trichloropropane	77443	96–18–4	Fumigant contaminant, paint and varnish remover	Agency for Toxic Substances and Disease Registry, 1992a; Tesoriero and others, 2001.
SH2020	3-Chloro-1-propene	78109	107–05–1	Fumigant contaminant	Cohen and others, 1983; U.S. National Library of Medicine, 2006.
SH2020	Acrylonitrile	34215	107–13–1	Fumigant, pesticide	Bender and others, 1999; Scorecard, 2006.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Organic synthesis compounds—Continued		
SH1433	Anthraquinone	62066	84–65–1	Bird repellant, 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.
SH1433	Carbazole	62071	86–74–8	Synthesis of dyes, combustion product	Budavari, 1989; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
SH2020	Carbon disulfide	77041	75–15–0	Solvent, syntheses, fumigant, sulfate-reduction product	Budavari, 1989; Megonigal and others, 2004; Scorecard, 2006.
SH2020	Chloromethane	34418	74–87–3	Blowing agent/propellant, solvent, refrigerant	Budavari, 1989; U.S. National Library of Medicine, 2006.
SH2020	Ethyl methacrylate (ethyl 2-methyl-2-propanoate)	73570	97–63–2	Hairspray, used to make polymers, chemical intermediate	Scorecard, 2006; U.S. National Library of Medicine, 2006.
SH2020	Hexachlorobutadiene	39702	87–68–3	Used in rubber manufacture, solvent, pesticide (non-U.S.)	Bender and others, 1999; California Environmental Protection Agency, 1999.
SH2020	Iodomethane	77424	74–88–4	Microscopy, circuit board manufacture, fire extinguishers, proposed fumigant	Budavari, 1989; U.S. Environmental Protection Agency, 2006.
SH2020	Methyl acrylate (methyl-2-propenoate)	49991	96–33–3	Manufacture of resins, paper, plastic	Budavari, 1989; U.S. National Library of Medicine, 2006.
SH2020	Methyl acrylonitrile (2-methyl-2-propenenitrile)	81593	126–98–7	Organic synthesis, polymer manufacture, chemical intermediate	Budavari, 1989; United Nations Environmental Programme, 2002; U.S. National Library of Medicine, 2006.
SH2020	Methyl methacrylate (methyl 2-methyl-2-propenoate)	81597	80–62–6	Manufacture of paint, paper, acrylic, chemical intermediate, pesticide adjuvant	U.S. National Library of Medicine, 2006; U.S. Environmental Protection Agency, 2009; Spectrum Laboratories Inc., 2010a.
SH2020	*trans*-1,4-Dichloro-2-butene	73547	110–57–6	Chemical intermediate	U.S. National Library of Medicine, 2006.
SH2020	Vinyl bromide	50002	593–60–2	Plastic manufacture, 1,2-dibromoethane degradate, flame retardant	Barbash and Reinhard, 1989; Bender and others, 1999.
SH2020	Vinyl chloride	39175	75–01–4	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.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Pavement- and combustion-derived compounds		
SH1433	Anthracene	34221	120–12–7	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.
SH1433	Benzo[a]pyrene	34248	50–32–8	Polynuclear aromatic hydrocarbon, cancer research chemical	Zaugg and others, 2002, Glassmeyer and others, 2005.
SH1433	Fluoranthene	34377	206–44–0	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.
SH1433	Phenanthrene	34462	85–01–8	Polynuclear aromatic hydrocarbon, manufacture of dyes, explosives, and drugs, used in research	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Pyrene	34470	129–00–0	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		
SH1433	3-*tert*-Butyl-4-hydroxy anisole (BHA)	62059	25013–16–5	Antioxidant, preservative, food packaging, and rubber and petroleum products	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	4-Cumylphenol	62060	599–64–4	Nonionic detergent metabolite	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	4-*n*-Octylphenol	62061	1806–26–4	Nonionic detergent metabolite	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	4-*tert*-Octylphenol	62062	140–66–9	Nonionic detergent metabolite	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Acetophenone	62064	98–86–2	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.
SH1433	Acetyl hexamethyl tetrahydronaphthalene (AHTN)	62065	21145–77–7	Widely used musk fragrance	Zaugg and others, 2002.
SH1433	Benzophenone	62067	119–61–9	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.
SH2020	Bromochloromethane	77297	74–97–5	Fire extinguishing fluid, intermediate in pesticide manufacturing	Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2060	Caffeine	50305	58–08–2	Beverage ingredient, diuretic	Furlong and others, 2001; Glassmeyer and others, 2005.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
				Personal-care and domestic-use products—Continued	
SH1433	Camphor	62070	76–22–2	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, 2010; Glassmeyer and others, 2005.
SH1433	Cotinine	62005	486–56–6	Primary nicotine metabolite, nonprescription drug	Kolpin and others, 2002; Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	*d*-Limonene	62073	5989–27–5	Antimicrobial, fragrance	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Hexahydrohexamethyl-cyclopentabenzo-pyran (HHCB)	62075	1222–05–5	Widely used musk fragrance	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Indole	62076	120–72–9	Pesticide adjuvant, coffee ingredient, fragrance	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH1433	Isoborneol	62077	124–76–5	Flavorant, fragrance, disinfection ingredient	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. National Library of Medicine, 2006.
SH1433	Isoquinoline	62079	119–65–3	Flavors and fragrances	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Menthol (5-methyl-2-[1-methylethyl] cyclohexanol)	62080	89–78–1	Cigarettes, cough drops, liniment, mouthwash	Zaugg and others, 2002.
SH1433	Methyl salicylate	62081	119–36–8	Analgesic, decongestant, toilet and window cleaner	Kolpin and others, 2002; Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006.
SH1433	N,N-diethyl-*meta*-toluamide (DEET)	62082	134–62–3	Insect repellent	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Nonylphenol, diethoxy- (total)	62083	26027–38–2	Nonionic detergent metabolite	Zaugg and others, 2002.
SH1433	Octylphenol, diethoxy- (OPEO2)	61705	--	Nonionic detergent metabolite	Zaugg and others, 2002.
SH1433	Octylphenol, mono-ethoxy- (OPEO1)	61706	--	Nonionic detergent metabolite	Zaugg and others, 2002.
SH1433	*para*-Nonylphenol (total)	62085	84852–15–3	Surfactant intermediate	Zaugg and others, 2002; Glassmeyer and others, 2005.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Personal-care and domestic-use products—Continued		
SH1433	Phenol	34466	108–95–2	Disinfectant	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Triclosan	62090	3380–34–5	Antimicrobial, preservative for cosmetics and detergents preparations	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Triethyl citrate	62091	77–93–0	Cosmetics, pharmaceuticals, plasticizer	Zaugg and others, 2002; Glassmeyer and others, 2005; U.S. National Library of Medicine, 2006.
			Plant- or animal-derived biochemicals		
SH1433	3-*beta*-Coprostanol	62057	360–68–9	Fecal indicator (carnivores)	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	3-Methyl-1(H)-indole (Skatole)	62058	83–34–1	In animal waste, stench in feces, in coal tar	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	*beta*-Sitosterol	62068	83–46–5	Plant sterol	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	*beta*-Stigmastanol	62086	19466–47–8	Plant sterol	Zaugg and others, 2002; Glassmeyer and others, 2005.
SH1433	Cholesterol	62072	57–88–5	Fecal indicator, plant sterol	Zaugg and others, 2002; Glassmeyer and others, 2005.
			Refrigerants and propellants		
SH2020	1,1,2-Trichloro-1,2,2-trifluoroethane (CFC–113)	77652	76–13–1	Electroplating, degreasing, adhesives, textiles, pesticide adjuvant	Bender and others, 1999; CambridgeSoft Corporation, 2010; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	Dichlorodifluoromethane (CFC–12)	34668	75–71–8	Insulation, inhalers, insecticide, pesticide adjuvant	Bender and others, 1999; CambridgeSoft Corporation, 2010; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	Trichlorofluoromethane (CFC–11)	34488	75–69–4	Hairspray, inhalers, insecticide, pesticide adjuvant	Bender and others, 1999; CambridgeSoft Corporation, 2010; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
			Solvents		
SH2020	1,1,1,2-Tetrachloroethane	77562	630–20–6	Solvent for varnish	Bender and others, 1999; Scorecard, 2006.
SH2020	1,1,1-Trichloroethane	34506	71–55–6	Electronics, pharmaceutical manufacture, degreaser; pesticide adjuvant, fumigant	Bender and others, 1999; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	1,1,2,2-Tetrachloroethane	34516	79–34–5	Manufacture of solvents, insecticide, pesticide adjuvant	Bender and others, 1999; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	1,1,2-Trichloroethane	34511	79–00–5	Aerosol paints, manufacture solvent	Bender and others, 1999; Scorecard, 2006.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Solvents—Continued		
SH2020	1,1-Dichloroethane	34496	75–34–3	Lubricant, cleaner; anaerobic 1,1,1-trichloroethane degradate	Klecka and others, 1990; Bender and others, 1999; Scorecard, 2006.
SH2020	1,1-Dichloroethene	34501	75–35–4	1,1,1-trichloroethane degradate (aerobic); pharmaceutical solvent	Haag and Mill, 1988; Bender and others, 1999; Scorecard, 2006.
SH2020	1,2,4-Trichlorobenzene	34551	120–82–1	Manufacture of solvents; insecticide	Bender and others, 1999; Scorecard, 2006.
SH2020	1,2-Dichlorobenzene (*o*-dichlorobenzene)	34536	95–50–1	Disinfectant, deodorant, consumer solvent	Bender and others, 1999; Scorecard, 2006.
SH2020	1,2-Dichloroethane (ethylene dichloride)	32103	107–06–2	Fumigant, manufacture of solvents, anti-knock compound in gasoline	Bender and others, 1999; National Oceanic and Atmospheric Administration, 2008; Scorecard, 2006.
SH2020	1,3-Dichlorobenzene (*m*-dichlorobenzene)	34566	541–73–1	Organic synthesis, fumigant	Bender and others, 1999.
SH2020	2-Chlorotoluene	77275	95–49–8	Pesticide adjuvant	Bender and others, 1999; U.S. Environmental Protection Agency, 2009.
SH2020	2-Hexanone	77103	591–78–6	Organic synthesis	Agency for Toxic Substances and Disease Registry, 1992b; Spectrum Laboratories Inc., 2010b.
SH2020	4-Chlorotoluene	77277	106–43–4	Pesticide adjuvant	Bender and others, 1999; U.S. Environmental Protection Agency, 2009.
SH2020	Acetone (2-propanone)	81552	67–64–1	Organic synthesis, chemical intermediate, pesticide adjuvant	Budavari, 1989; U.S. Environmental Protection Agency, 2009.
SH2020	Bromobenzene	81555	108–86–1	Organic synthesis, additive to oil	Bender and others, 1999; U.S. National Library of Medicine, 2006.
SH2020	Carbon tetrachloride	32102	56–23–5	Fumigant, solvent	Bender and others, 1999; Scorecard, 2006.
SH2020	Chlorobenzene	34301	108–90–7	Disinfectant, herbicide, building materials, solvent	Budavari, 1989; Bender and others, 1999; Scorecard, 2006.
SH2020	Chloroethane	34311	75–00–3	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.
SH2020	*cis*-1,2-Dichloroethene	77093	156–59–2	Trichloroethene degradate (anaerobic)	Bender and others, 1999; Lorah and Olsen, 1999.
SH2020	Dibromomethane	30217	74–95–3	Organic synthesis (pesticide manufacture), heavy liquid for mineral separations, fire extinguishers	Bender and others, 1999.
SH2020	Diethyl ether (1,1’-oxybisethane)	81576	60–29–7	Detergent, solvent, pharmaceuticals, cosmetics	Budavari, 1989; Scorecard, 2006.

Appendix 1. Compounds analyzed in Source Water-Quality Assessment studies by primary use or source groups.—Continued

[USGS, U.S. Geological Survey; CASRN, Chemical Abstracts Service Registry Number®; --, no additional information]

USGS analytical schedule	Compound name (abbreviation or other name)	USGS parameter code	CASRN[a]	Secondary uses or sources	References for use and source information
			Solvents—Continued		
SH2020	Hexachloroethane	34396	67–72–1	Lubricant, dry cleaning solvent	Budavari, 1989; Scorecard, 2006.
SH1433	Isophorone	34409	78–59–1	Herbicide, adjuvant, solvent	Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006; U.S. Environmental Protection Agency, 2009; U.S. National Library of Medicine, 2006.
SH4024	Methyl acetate	77032	79–20–9	Aerosol paints	Scorecard, 2006.
SH2020	Methyl ethyl ketone (MEK)	81595	78–93–3	Adjuvant, solvent, cleaners, polyvinyl chloride (PVC) glue and primer	Bender and others, 1999; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	Methyl isobutyl ketone (MIBK) (4-methyl-2-pentanone)	78133	108–10–1	Solvent, personal care products, insecticide, pesticide adjuvant, polyvinyl chloride (PVC) glue	Budavari, 1989; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	Methylene chloride	34423	75–09–2	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.
SH2020	*n*-Propylbenzene	77224	103–65–1	Insulation, flooring manufacture	Bender and others, 1999; Scorecard, 2006.
SH1433	*p*-Cresol	62084	106–44–5	Paint/varnish removal, solvent, disinfectant, chemical intermediate for synthetic resins	Budavari, 1989; Zaugg and others, 2002; Glassmeyer and others, 2005; Scorecard, 2006.
SH2020	Perchloroethene (PCE; tetrachloroethene)	34475	127–18–4	Fumigant, solvent	Bender and others, 1999; Glassmeyer and others, 2005; Scorecard, 2006.
SH2020	Tetrahydrofuran (1,4-epoxybutane)	81607	109–99–9	Adjuvant, cleaners, solvent, polyvinyl chloride (PVC) glue and primer	Budavari, 1989; Scorecard, 2006; U.S. Environmental Protection Agency, 2009.
SH2020	*trans*-1,2-Dichloroethene	34546	156–60–5	Trichloroethene degradate	Bender and others, 1999; Lorah and Olsen, 1999.
SH2020	Trichloroethene (TCE)	39180	79–01–6	Fumigant, solvent, anaerobic perchloroethene degradate	Vogel and McCarty, 1985; Bender and others, 1999; Scorecard, 2006.

[a]This report contains CASRNs, which is a Registered Trademark of the American Chemical Society. The Chemical Abstracts Service (CAS) recommends the verification of the CASRNs through CAS Client Services[SM].

[b]Letter prefix added to CASRN because CASRN not available for *cis*- or *trans*-isomers.

Appendix 2. Concentrations of anthropogenic organic compounds in groundwater and associated finished water from community water systems and in quality-assurance samples for Source Water-Quality Assessment studies, 2002–10

The Microsoft Excel spreadsheet (*gwdata.xls*) contains a worksheet (worksheet: Documentation and abbreviations) that describes the documentation and abbreviations used in Appendix 2. The spreadsheet also contains concentration data and quality-assurance/quality-control data for each use (or source) group in separate worksheets named as follows:

1. Disinfection by-products (worksheet: Disinfection by-products)
2. Fumigant-related compounds (worksheet: Fumigant-related compounds)
3. Fungicides and fungicide degradates (worksheet: Fungicides)
4. Gasoline hydrocarbons, oxygenates, and oxygenate degradates (worksheet: Gasoline hydrocarbons)
5. Herbicides and herbicide degradates (worksheet: Herbicides)
6. Insecticides and insecticide degradates (worksheet: Insecticides)
7. Manufacturing additives (worksheet: Manufacturing additives)
8. Organic synthesis compounds (worksheet: Organic synthesis compounds)
9. Pavement- and combustion-derived compounds (worksheet: Pavement- & combustion-derived)
10. Personal-care and domestic-use products (worksheet: Personal-care products)
11. Plant- or animal-derived biochemicals (worksheet: Plant- or animal-derived biochem)
12. Refrigerants and propellants (worksheet: Refrigerants and propellants)
13. Solvents (worksheet: Solvents)

A tab-delimited text file (*Appendix2_readme.txt*) describes the documentation and abbreviations used in Appendix 2. A tab-delimited text file for concentration data is presented for each use (or source) group as follows:

1. Disinfection by-products (*gw_byprod.txt*)
2. Fumigant-related compounds (*gw_fumigant.txt*)
3. Fungicides and fungicide degradates (*gw_fungicide.txt*)
4. Gasoline hydrocarbons, oxygenates, and oxygenate degradates (*gw_gashydrocarb.txt*)
5. Herbicides and herbicide degradates (*gw_herbicide.txt*)
6. Insecticides and insecticide degradates (*gw_insecticide.txt*)
7. Manufacturing additives (*gw_manufact.txt*)
8. Organic synthesis compounds (*gw_orgsyn.txt*)
9. Pavement- and combustion-derived compounds (*gw_pavement.txt*)
10. Personal-care and domestic-use products (*gw_personal.txt*)
11. Plant- or animal-derived biochemicals (*gw_biochem.txt*)
12. Refrigerants and propellants (*gw_refrig.txt*)
13. Solvents (*gw_solvent.txt*)

Appendix 3. Concentrations of anthropogenic organic compounds in surface water and associated finished water from community water systems and in quality-assurance samples for Source Water-Quality Assessment studies, 2002–10

The Microsoft Excel spreadsheet (*swdata.xls*) contains a worksheet (worksheet: Documentation and abbreviations) that describes the documentation and abbreviations used in Appendix 3. The spreadsheet also contains concentration and quality-assurance/quality-control data for surface water and the associated finished water for each use (or source) group in separate worksheets named as follows:

1. Disinfection by-products (worksheet: Disinfection by-products)
2. Fumigant-related compounds (worksheet: Fumigant-related compounds)
3. Fungicides and fungicide degradates (worksheet: Fungicides)
4. Gasoline hydrocarbons, oxygenates, and oxygenate degradates (worksheet: Gasoline hydrocarbons)
5. Herbicides and herbicide degradates (worksheet: Herbicides)
6. Insecticides and insecticide degradates (worksheet: Insecticides)
7. Manufacturing additives (worksheet: Manufacturing additives)
8. Organic synthesis compounds (worksheet: Organic synthesis compounds)
9. Pavement- and combustion-derived compounds (worksheet: Pavement- & combustion-derived)
10. Personal-care and domestic-use products (worksheet: Personal-care products)
11. Plant- or animal-derived biochemicals (worksheet: Plant- or animal-derived bioche)
12. Refrigerants and propellants (worksheet: Refrigerants and propellants)
13. Solvents (worksheet: Solvents)

A tab-delimited text file (*Appendix3_readme.txt*) describes the documentation and abbreviations used in Appendix 3. A tab-delimited text file for concentration data is presented for each use (or source) group as follows:

1. Disinfection by-products (*sw_byprod.txt*)
2. Fumigant-related compounds (*sw_fumigant.txt*)
3. Fungicides and fungicide degradates (*sw_fungicide.txt*)
4. Gasoline hydrocarbons, oxygenates, and oxygenate degradates (*sw_gashydrocarb.txt*)
5. Herbicides and herbicide degradates (*sw_herbicide.txt*)
6. Insecticides and insecticide degradates (*sw_insecticide.txt)*
7. Manufacturing additives (*sw_manufact.txt*)
8. Organic synthesis compounds (*sw_orgsyn.txt*)
9. Pavement- and combustion-derived compounds (*sw_pavement.txt*)
10. Personal-care and domestic-use products (*sw_personal.txt*)
11. Plant- or animal-derived biochemicals (*sw_biochem.txt*)
12. Refrigerants and propellants (*sw_refrig.txt*)
13. Solvents (*sw_solvent.txt*)

Publishing support provided by:
Rolla Publishing Service Center

For more information concerning this publication, contact:
Director, USGS South Dakota Water Science Center
1608 Mountain View Road, Rapid City, SD 57702
(605) 394-3200
http://sd.water.usgs.gov/

Information regarding the National Water-Quality Assessment Program is available at:
http://water.usgs.gov/nawqa/

Carter and others—**Concentration Data for Anthropogenic Organic Compounds in Groundwater, Surface Water, and Finished Water**—Data Series 544