

# (WERF) Trace Organic Compounds (TOrcs) database

**Manage and screen high priority trace organic compound exposure and effects data**

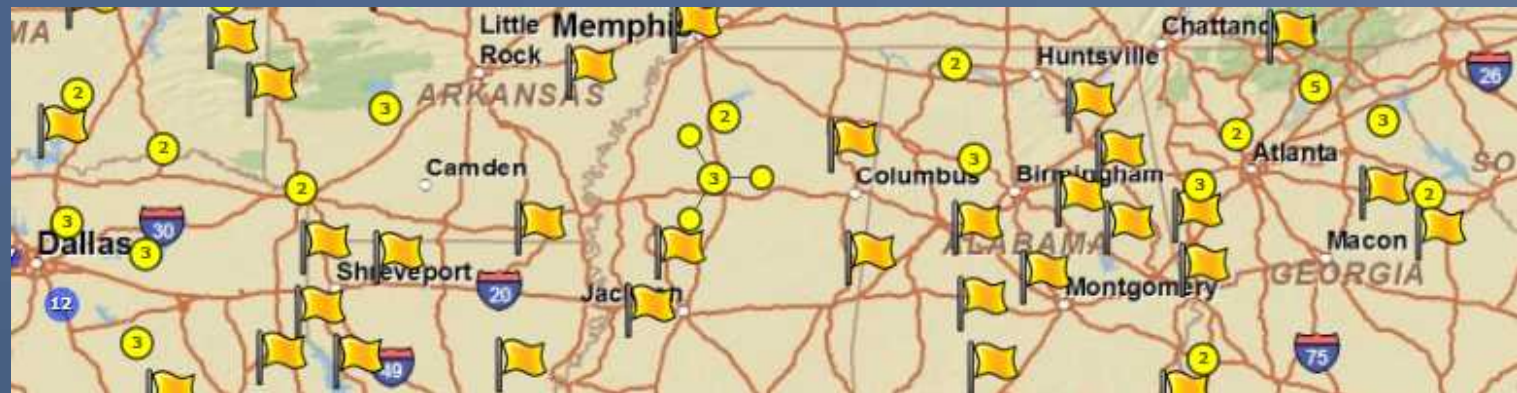
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Jerry Diamond  
Tetra Tech, Inc.**

# What are Trace Organic Compounds?

- Trace organic compounds (TOrcs) include pharmaceuticals, personal care products, surfactants, pesticides, flame retardants, and others.
- Also known as Contaminants of Emerging Concern (CEC).
- Most TOrcs are not well studied or regulated, though more information is becoming available as analysis techniques improve.

## Purpose Of WERF's TOrC Database

- Provide a user-friendly tool that allows users to search available TOrC data in river basins and lakes across the country.
- Search for data regarding a specific TOrC.
- Download TOrC data and compare results.
- Begin to relate TOrC concentrations and biological data, where available.

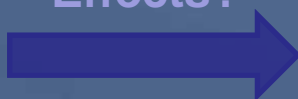


# Future Tools And Applications Of WERF's TOrC Database

- Search by groups of chemicals (i.e. surfactants, flame retardants, nonylphenols, etc.) rather than individual compounds.
- Group chemicals with similar properties (i.e. estrogens) to evaluate possible additive biological effects at sites.
- Support development of tools for WWTPs, resource agencies, and water quality specialists to begin to diagnose whether TOrCs cause or have the potential to cause aquatic ecological effects.




Effects?



## The Database is not Designed to:

- Perform Sophisticated GIS Analyses.
  - The map tool in the database is intended as a browsing tool. However TOrC data can be downloaded and used in your spatial analysis program to link TOrC data with land use, permitted discharges, etc.
- Make Cause-and-Effect Statements About TOrCs and Biological Endpoints.
  - More biological data and information about habitat and other factors are necessary to determine if TOrCs could be responsible for an observed biological impairment.



Chemical						
Biological		Habitat				
Compound	CAS	Result	Unit	Endocrine?	Sample Date Range	Media Type
1,4-Dichlorobenzene	106-46-7	0.06	ug/l	No	6/3/2000 - 6/3/2000	Water

# Who Could Benefit From WERF's TOrC Database?

- Academic researchers
- Federal and state agencies
- NGOs interested in water quality
- Consulting and engineering firms

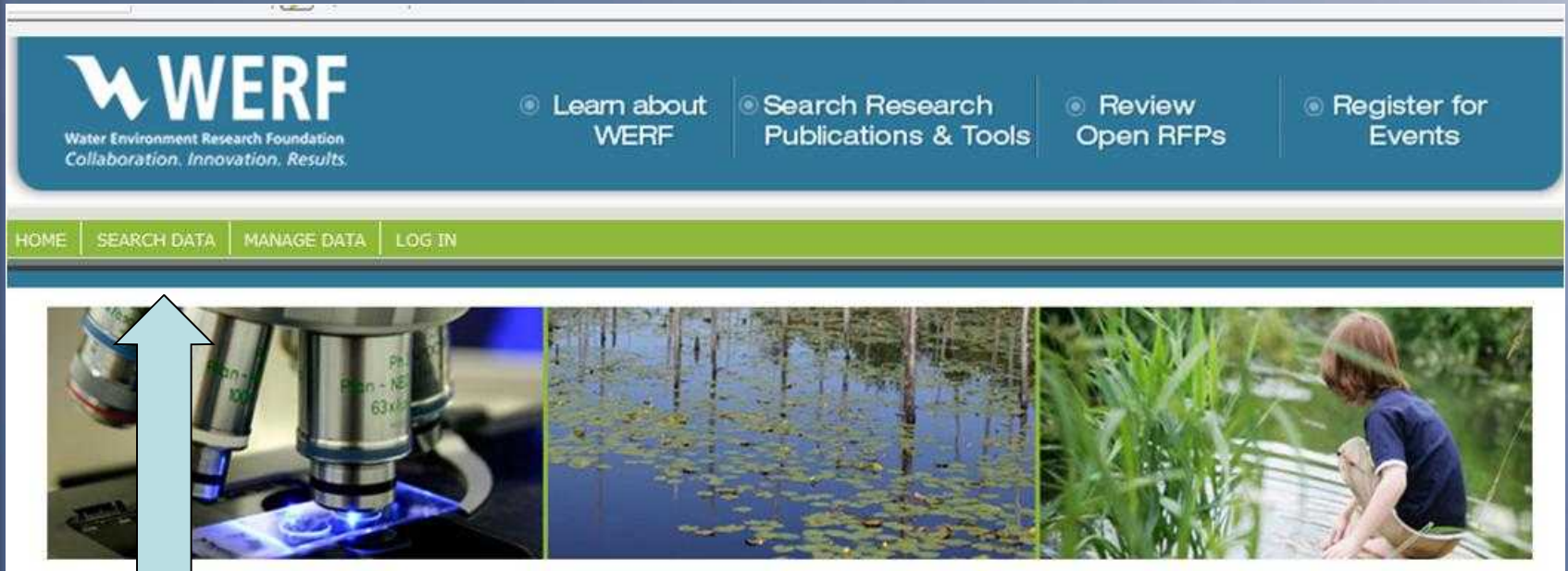


Compound	CAS	Result	Unit	Endocrine?	Sample Date Range	Media Typ
Phenol	108-95-2	25	ug/kg	No	4/1/2004 - 9/9/2004	Tissue-Pla ▲
d-limonene	5989-27-5	152	ug/kg	No	4/1/2004 - 9/9/2004	Tissue-Pla
Acetophenone	98-86-2	25	ug/kg	No	4/1/2004 - 9/9/2004	Tissue-Pla
Naphthalene	91-20-3	41.9	ug/kg	No	4/1/2004 - 9/9/2004	Tissue-Pla
2-Methylnaphthalene	91-57-6	47.1	ug/kg	No	4/1/2004 - 9/9/2004	Tissue-Pla ▼

# The home page - <http://traceorganicsecotool.werf.org/>

The screenshot shows the website interface within a Windows Internet Explorer browser window. The address bar displays the URL <http://traceorganicsecotool.werf.org/>. The browser's menu bar includes File, Edit, View, Favorites, Tools, and Help. The Favorites bar shows 'WERF' and 'Sign out'. The search bar contains the text 'WERF'. The main navigation bar is dark blue and features the WERF logo (Water Environment Research Foundation) and three menu items: 'Learn about WERF', 'Search Research Publications & Tools', and 'Review Open RFPs'. A secondary navigation bar is light green and contains 'HOME', 'SEARCH DATA', 'MANAGE DATA', and 'LOG IN'. Below this is a banner with three images: a microscope, a pond with lily pads, and a person in a field. A light blue arrow points to the 'SEARCH DATA' link. A blue starburst graphic with the text 'Explore Data' is overlaid on the right side. At the bottom left, a red link says 'Click here if you want to submit comments and/or suggestions.'. The status bar at the bottom shows 'Internet | Protected Mode: On' and '115%' zoom.

# Search the Database



Click on  
'SEARCH DATA'

## Search the Database for:

- Trace Organic Chemical
- Water Body of Interest
- Biological Endpoints



# Home Page for the Map



Water Environment Research Foundation  
Collaboration. Innovation. Results.

Learn about  
WERF

Search Research  
Publications & Tools

Review  
Open RFPs

Reg

HOME | SEARCH DATA | MANAGE DATA | LOG OFF JFLIPPIN2011



# Map Interface Tools

The screenshot shows the WERF website interface. At the top, there is a navigation bar with the WERF logo and links for 'Learn about WERF', 'Search Research Publications & Tools', 'Review Open RFPs', and 'Register for Events'. Below this is a secondary navigation bar with 'HOME', 'SEARCH DATA', 'MANAGE DATA', and 'LOG OFF JFLIPPIN2011'. The main content area features a map of North America with various site markers. A red box highlights a navigation tool in the top left corner. Another red box highlights a 'Map Tools' menu in the top center, which includes icons for 'Map', 'Tools', and 'Help'. A third red box highlights a search tool in the top right corner. A callout box labeled 'Map Options' points to the 'Map Tools' menu. A callout box labeled 'Navigation Tool' points to the navigation tool in the top left. A callout box labeled 'Search Tools' points to the search tool in the top right. A callout box labeled 'Map Key' points to a legend in the bottom left, which shows four colored circles (blue, light blue, yellow, and green) with numbers inside, representing the number of sites within an area. A callout box labeled 'Individual site' points to a yellow flag icon on the map, representing an individual site. The map itself shows various cities and states, with site markers in different colors and sizes. The bottom of the page has a footer with 'Water Environm...', 'Alexandria, VA 22314', '571.384.2100', and 'email.us'.



# Browsing the database using the map interface

Study Info:  
Title, Authors,  
Location



Click on Flag  
for More  
Information

Water-quality data for pharmaceuticals, hormones, and other organic wastewater contaminants in US streams 1999-2000  
Barnes KK, Kolpin DA, Meyer MT, Thurman EM, Furlong ET, Zaugg SD, and Barber LB  
USGS  
Des Plaines River at Riverside, IL  
River/Stream  
Illinois  
41°49'19"N, 87°49'16"W  
5/19/1999 - 9/6/2000

Chemical Biological Habitat

Compound	CAS	Result	Unit	Endocrine? ▾	Sample Date Range	Media Type	Trace
4-Octylphenol monoethoxylate	26636-32-8	0.1	ug/l	Yes	5/19/1999 - 9/6/2000	Water	
4-Nonylphenol	25154-52-3	0.8	ug/l	Yes	5/19/1999 - 9/6/2000	W----	
Bisphenol A	80-05-7	0.5	ug/l	Yes	5/19/1999 - 9/6/2000	W	
Diethyl phthalate	84-66-2	0.25	ug/l	Yes	5/19/1999 - 9/6/2000	W	
Carbaryl	63-25-2	0.06	ug/l	Yes	5/19/1999 - 9/6/2000	W	

Site  
Measurements :  
TOrcs

Biology and Habitat  
information may also  
be available

# Map Options



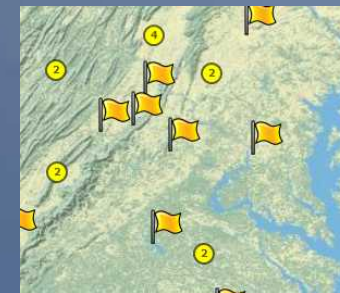
View Other Map Types



Street Map

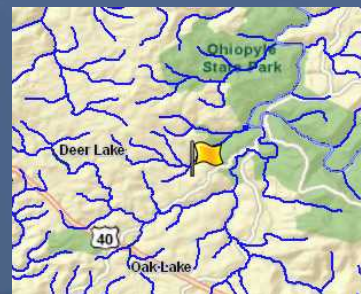


Satellite Map



USGS Map

Add Map Layers



National Hydrography Dataset



Watershed Boundaries

# Support for multiple sample and media types

A Reconnaissance for Emerging Contaminants in the South Branch Potomac River, Cacapon River, and Williams River  
 Chambers, DB, Leiker, TJ  
 USGS  
 Williams River at Dyer, WV  
 River/Stream  
 West Virginia  
 38°22'44"N, 80°29'02"W  
 4/1/2004 - 4/1/2004

Chemical   Biological   Habitat

Compound	CAS	Resu	Unit	Endocr	Sample Date Range	Media Type
Diethyl phthalate	84-66-2	94	ug/kg	Yes	4/1/2004 - 4/1/2004	Tissue-Plasma
Diethyl phthalate	84-66-2	110	ug/kg	Yes	4/1/2004 - 4/1/2004	Tissue-Plasma
Diethyl phthalate	84-66-2	150	ug/kg	Yes	4/1/2004 - 4/1/2004	Tissue-Plasma
d-limonene	5989-27-5	69.8	ug/kg	No	4/1/2004 - 4/1/2004	Tissue-Plasma
d-limonene	5989-27-5	32.8	ug/kg	No	4/1/2004 - 4/1/2004	Tissue-Plasma

# Multiple ways to search and download data

The image displays a web application interface for searching and downloading data. It is divided into three main sections:

- Search Filters (Top Left):** A panel with several checkboxes for filtering data: "Published?", "Primary?", "Has been QA/QC?", "Has quality of Coordinates?", and "Endocrine disrupting compound?". Below these are two date input fields with the format "<M/d/yyyy>" and the value "15". "Find" and "Clear" buttons are at the bottom.
- Search Methods (Top Right):** A panel with three dropdown menus: "Select sites near an address", "Select sites in a Hydrological Unit Code", and "Select sites using map". "Find" and "Clear" buttons are at the bottom.
- Map (Bottom):** A map of the United States with various cities marked by yellow flags and numbered circles (1-15). A search panel is overlaid on the right side of the map.

**Search Panel (Bottom Right):** A panel with radio buttons for "Compound", "CAS", "Habitat", and "Taxonomy". A search input field contains "Lindane". "Add", "Remove", and "Clear" buttons are below the input. A list of results shows "Estriol" and "Lindane". "Find" and "Clear" buttons are at the bottom.

Two large light blue arrows point from the text "Search tools available from the Map interface." to the search filters and search methods panels.

# Download the Results of Your Search



Click "Summary"  
and download  
will begin for  
selected sites



The screenshot shows a Windows Internet Explorer browser window displaying the WERF website. A download dialog box is open, titled "11% of summary\_report.xls from werf2.tetrach-ff...". The dialog box shows the file name "summary\_report.xls from werf2.tetrach-ff.com", the estimated time left (3 min 49 sec), the download location (C:\Projects\summary\_report.xls), and the transfer rate (24.6KB/Sec). There are "Open", "Open Folder", and "Cancel" buttons. A SmartScreen Filter notification is also visible at the bottom of the dialog box.

Select sampling sites using the map and download to a spreadsheet.

Taxonomy	Count	Exclude	Sample Date Range
Turbellaria	15	No	7/24/2002 - 7/24/2002
Oligochaeta	37	No	7/24/2002 - 7/24/2002
Gyraulius	2	No	7/24/2002 - 7/24/2002
Baetis tricaudatus	27	No	7/24/2002 - 7/24/2002
Laccobius	1	No	7/24/2002 - 7/24/2002
Limnolia	8	No	7/24/2002 - 7/24/2002

# Downloaded Data

- **Information in Spreadsheet Tabs:**
- **Study Summary:** Title, Authors, Number of Locations, Number of Sampling Events, Number of Results.
- **Result Summary:** Summary statistics for compounds in the selected studies; Frequency of Detection, Min, Max, Average, Median, Mean.
- **Study Results, Location Results, Sampling Results, Chemical Results:** Original data from studies; specifics for each study, site coordinates, sampling dates, etc.

summary\_report[1].xls [Protected View] - Microsoft Excel

Protected View This file originated from an Internet location and might be unsafe. Click for more details. Enable Editing

A2 Title

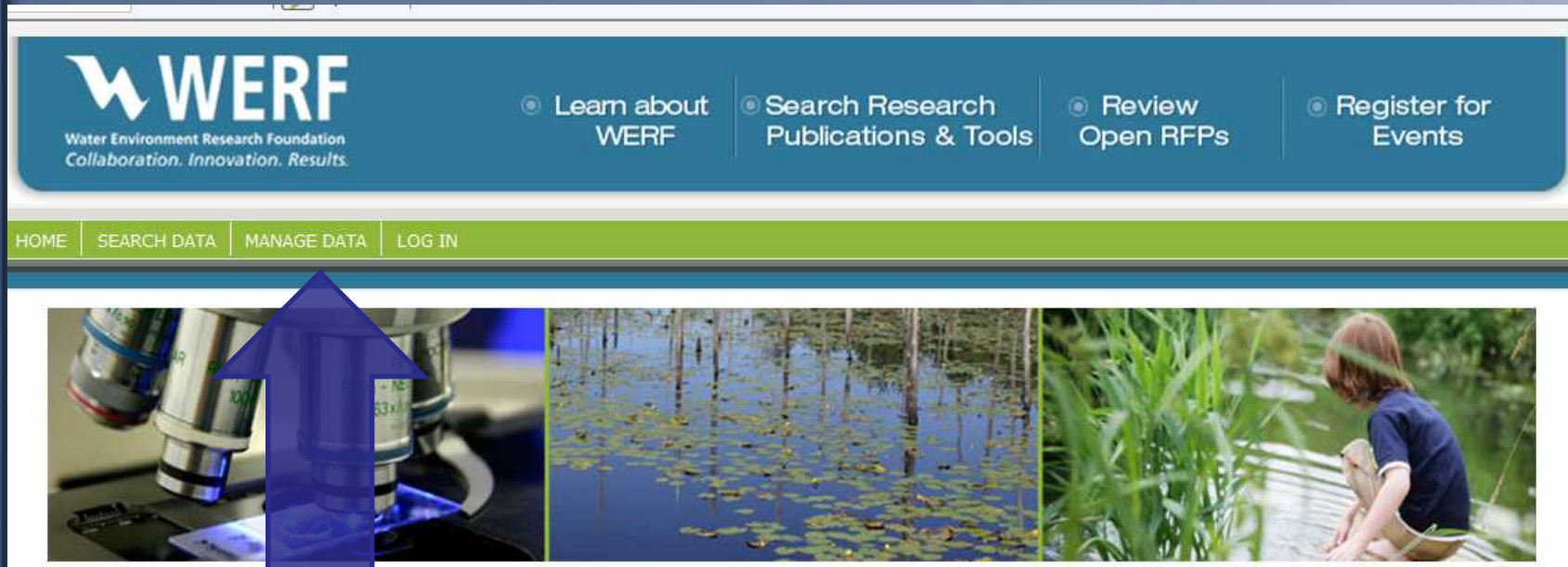
	A	B	C	D	E	F	G	H
1	Study Summary							
2	Title	Primary Author	Organization	Status	Sampling Date Range	# of Locations	# of Sampling Events	# of Results
3	King County Surface Water Quality	King County, Department of	King County	Published	10/7/2002 - 5/26/2004	87	410	13374
4	Occurrence of endocrine active compounds and biological responses in the Mississippi R	Lee, K.E.	USGS	Published	6/26/2006 - 7/20/2006	41	41	2952
5	Occurrence of organic wastewater compounds in wastewater effluent and the Big Sioux Sando, S.K.		USGS	Published	8/18/2003 - 6/18/2004	18	37	3510
6	Water-quality data for pharmaceuticals, hormones, and other organic wastewater contami	Barnes KK	USGS	Published	4/3/1999 - 10/5/2000	139	729	15936
7	Reproductive Disruption in Fish Downstream from an Estrogenic Wastewater Effluent	Vajda AM	University of Colorado, USG	Published	9/3/2003 - 9/6/2003	3	6	102
8	Pharmaceuticals, Hormones, and Other Organic Wastewater Contaminants in U.S. Stream	Kolpin, DW	U.S. Geological Survey	Published	4/23/1999 - 10/3/2000	19	22	1363
9	Occurrence and distribution of steroids, hormones, and selected pharmaceuticals in Sout	Singh, SP	Florida International Universi	Published	1/1/2004 - 7/9/2004	3	3	62
10	Concentrations of selected pharmaceuticals and antibiotics in south-central Pennsylvania	Loper, CA	USGS	Published	3/23/1993 - 7/21/2009	28	249	9295
11	Comprehensive Water Quality of the Boulder Creek Watershed, Colorado, During High-Fl	Murphy, SF	USGS	Published	5/8/1972 - 4/19/2005	4	21	261
12								
13								
14								
15								
16								
17								
18								
19								

Study Summary Result Summary Chemical Summary Study Results Location Results Sampling Results Chemical Result[1]

Ready 100%

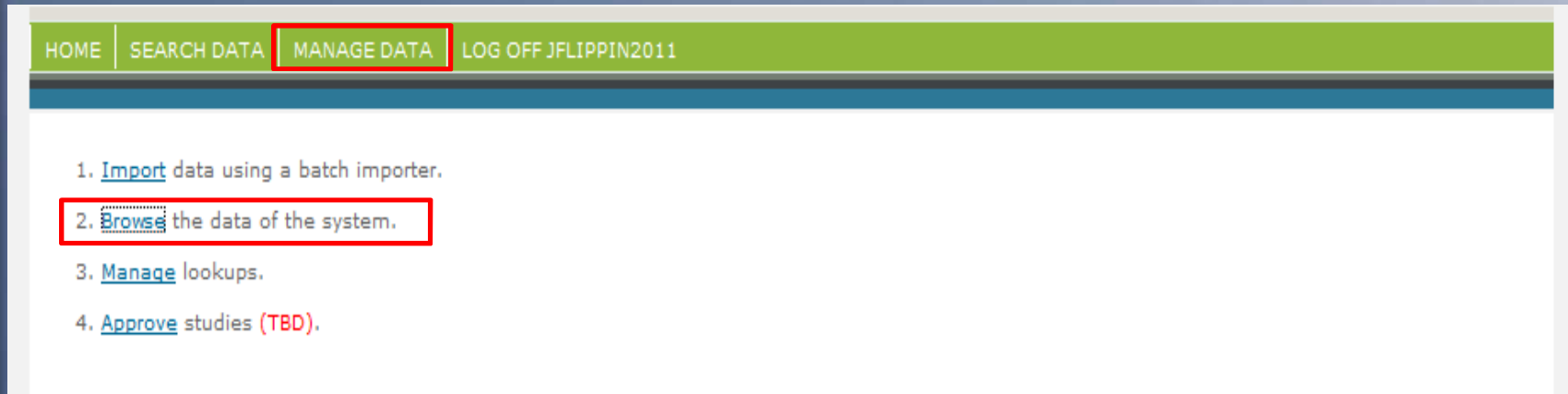


# Manage the Database



- Search for Lists of Studies in Database
- Add New Studies to the Database
- Requires an Account

# Search the Database for Study Information



The screenshot shows a web application interface with a green navigation bar at the top. The navigation bar contains the following items: HOME, SEARCH DATA, MANAGE DATA (highlighted with a red box), and LOG OFF JFLIPPIN2011. Below the navigation bar, there is a list of actions:

1. [Import](#) data using a batch importer.
2. [Browse](#) the data of the system. (highlighted with a red box)
3. [Manage](#) lookups.
4. [Approve](#) studies (TBD).

Select “Manage Data”  
and then “Browse”







































# Search the Database for Study Information

Tabular list of studies in the database.

[Add Study](#) | [Import Studies](#)

Title      Primary Author      Keywords

Display 1 of 175 ➔

Action	Organization	Title	Primary Author	Status	Details	Monitoring Locations
 	Federal	Great Lake Study Pharmaceutical Compounds	IJCD	Preliminary		 (4)
 	Federal	Great Lake Study - Surfactants Compounds	Bennie et al 1997	Preliminary		 (38)
 	Federal	Great Lake Study - Surfactants Compounds	Kannan et al 2003	Preliminary		 (2)
 	Federal	Great Lake Study - Surfactants Compounds	Mayer et al 2007	Preliminary		 (1)
 	Federal	Great Lake Study - Surfactants Compounds	Rice et al 2003	Preliminary		 (8)
 	Puget Sound Stream Benthos Org.	Analyzing Stream Health	Puget Sound Stream Benthos Org.	Published		 (25)
 	King County	King County Surface Water Quality	King County, Department of Natural Resources and Parks	Published		 (87)
 	Trent University	Occurrence of Neutral and Acidic Drugs in the Effluents of Canadian Sewage Treatment Plants	Chris D. Metcalfe	Published		 (1)
 	American Water Resources Association	Estrogenic Compounds Downstream from Three Small Cities in Eastern Nebraska: Occurrence and Biological Effect	Marlo K. Sellin	Published		 (1)
 	USGS	A holistic passive integrative sampling approach for assessing the presence and potential impacts of waterborne environmental contaminants	J.D. Petty			

Click on "Monitoring Locations"  
There are 87 in the King County Dataset

# Search the Database for Study Information



Displaying 1 of 10 of 87

Action	Name	Type	Latitude	Longitude	Details	Sampling Events
 	0831	Major Lakes	47.51586111	-122.2190833		 (9)
 	0834	Major Lakes	47.61025	-122.2119167		 (4)
 	0817	Major Lakes	47.69483333	-122.2696389		 (4)
 	0804	Major Lakes	47.74676464	-122.2712373		 (6)
 	0807	Major Lakes	47.69894444	-122.2184722		 (4)
 	0614	Major Lakes	47.56232276	-122.0670647		 (7)

Site "0614" is one of 87 sites in the King County Dataset

Click on "Sampling Events."



























# Search the Database for Study Information

Study >> Location >> **Sampling Event**

[Add SamplingEvent](#) | [Import Sampling Events](#) | [Import Sample Types](#) | [Import Event Types](#)

Start Date:  End Date:  Sample Type:

Displaying 1 of 7 of 7

Action	Start Date	End Date	Sample Type	Details	Results
 	12/16/2002	12/16/2002	Sample-Routine		 (39)
 	12/16/2002	12/16/2002	Sample-Routine		 (39)
 	3/25/2003	3/25/2003	Sample-Routine		 (37)
 	3/25/2003	3/25/2003	Sample-Routine		 (37)
 	9/30/2003	9/30/2003	Sample-Routine		 (8)
 	12/15/2003	12/15/2003	Sample-Routine		 (8)
 	3/15/2004	3/15/2004	Sample-Routine		 (8)

Site 0614 has 7  
Sampling Events

Click on "Results"

# Search the Database for Study Information

Chemical Habitat Biological

Compound

Media Type

Measurement Type

-- Select --

-- Select --

Search

Displaying 1 of 10 of 39



Action	Compound	Media Type	Measurement Type	Data Qualifier	Converted Result	Original Result	Details
	1,2-dichlorobenzene	Water	Actual	<MDL			
	1,3-dichlorobenzene	Water	Actual	<MDL			
	1,4-Dichlorobenzene	Water	Actual	<MDL			
	2-Methylnaphthalene	Water	Actual	<MDL			
	4-methylphenol	Water	Actual	<MDL			
	Acenaphthene	Water	Actual	<MDL			
	Acenaphthylene	Water	Actual	<MDL			
	Aldrin	Water	Actual	<MDL			
	Anthracene	Water	Actual	<MDL			
	Bis(2-ethylhexyl)phthalate	Water	Actual	B	0.259 ug/l	0.259 ug/l	

The sample taken on 12/16/2002 has results for 39 chemical measurements.





# Add Data to WERF's Trace Organic Database

HOME | SEARCH DATA | MANAGE DATA | LOG OFF JFLIPPIN2011

1. [Import](#) data using a batch importer.
2. [Browse](#) the data of the system.
3. [Manage](#) lookups.
4. [Approve](#) studies (TBD).

Select "Manage Data"  
and then "Import"

# Add Your Data to WERF's Trace Organic Database

Name	Date modified	Type	Size
 Location.txt	5/9/2011 1:11 PM	TXT File	2 KB
 Results.txt	5/9/2011 1:18 PM	TXT File	3 KB
 Sampling Event.txt	5/9/2011 1:17 PM	TXT File	1 KB
 Study.txt	5/9/2011 1:02 PM	TXT File	1 KB

**Select Correctly  
Formatted File  
for Upload**



# Add Data to WERF's Trace Organic Database

WERF - Windows Internet Explorer  
http://werf2.tetrattech-ffx.com/BatchImport/GoToMapFields

HOME SEARCH DATA MANAGE DATA LOG OFF JWHITE

[Back to Previous Step](#)

## Step 1: Import Studies

Map the following fields before saving the data to the system

Study		Organization	
Study Id*	Study_ID	Name*	Organization
Title*	Title	Address Line 1	-- Select --
Primary Author*	Primary_Author	Address Line 2	-- Select --
Secondary Author	Secondary_Author	City	-- Select --
Year	-- Select --	State	-- Select --
Journal	-- Select --	Country	-- Select --
Volume	-- Select --	Zip Code	-- Select --
Pages	-- Select --	Phone	-- Select --
Original URL	-- Select --	Email	-- Select --
Published?	Published_Study_YN		
Primary?	-- Select --		
Has been QA/QC?	QA_QC_Study_YN		
Has quality of Coordinates?	Quality_of_Coordinates_YN		
Status*	Study_Status_ID		
Keywords*	Keywords		

Upload Details  
About the Study

# Update the Database with New Information



Upload the  
Location,  
Sampling Details,  
and Results of  
your Study

HOME | SEARCH DATA | MANAGE DATA | LOG OFF JWHITE

[Back to Previous Step](#)

### Step 2: Import Locations

Map the followig fields before saving the data to the system

**Location**

Study Id\*

Location Id\*

Name\*

Type\*

Description

Latitude\*

Longitude\*

Stream Name

NHD Stream Segment

HOME | SEARCH DATA | MANAGE DATA | LOG OFF JFLIPPIN2011

[Back to Previous Step](#)

### Step 3: Import Sampling Events

Map the followig fields before saving the data to the system

**Sampling Event**

Location Id\*

Sampling Event Id\*

Start Date\*

Start Time

End Date

End Time

Sample Type\*

Event Type

Comments

[Back to Previous Step](#)

### Step 4a: Import Chemical Results

Map the followig fields before saving the data to the system

**Result**

Sampling Event Id\*

Compound\*

Original Result Value\*

Original Result Value Unit\*

Measurement Type\*

Media Type\*

Media Subdivision Type

Save

# Update the Database with New Information

WERF - Windows Internet Explorer

http://werf2.tetrattech-ffx.com/SampleType

HOME SEARCH DATA MANAGE DATA LOG OFF JWWHITE

Manage Lookup: Sample Type

Submit Query

Sample Type

Name

Search Reset

Displaying 1 of 1

Action	Description	Reviewed?
		<input type="checkbox"/>
		<input type="checkbox"/>
		<input type="checkbox"/>
	MEASUREMENTS involve something measured in its environmental setting usually using some type of equipment. OBSERVATIONS are made by people, usually without the use of equipment, and are frequently qualitative.	<input type="checkbox"/>
	Measurements made in the field by an automated data logging device running unattended and producing a suite of data at repeating intervals by its owner/operator.	<input type="checkbox"/>
	A field activity conducted to evaluate a habitat, usually to an owner/operator defined habitat assessment.	<input type="checkbox"/>
	Sample-Routine	<input type="checkbox"/>
	Sample-Integrated Time Series	<input type="checkbox"/>
	Sample-Integrated Flow Proportioned	<input type="checkbox"/>
	Sample-Integrated Horizontal Profile	<input type="checkbox"/>
	Sample-Integrated Vertical Profile	<input type="checkbox"/>
	Sample-Integrated Cross-Sectional Profile	<input type="checkbox"/>
	Sample-Composite Without Parents	<input type="checkbox"/>

**Add new Compounds, Methods, Sample Types, etc to the Database**

<http://traceorganicsecotool.werf.org>



[www.werf.org](http://www.werf.org)

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Erich Emory – ORSANCO

Jim Pletl – HRSD

Elizabeth Toot-Levy – NEORSD

Tetra Tech

Jeffrey White

Vladi Royzman

Jerry Diamond