ISRP Chemical Substances Identifiers - User Guide

Table of contents

About

What is the Chemical Substances Identifiers web page?

The web page was created for the Iowa Superfund Research Program to provide downloadable tables listing substance identifier(s) for select PCB congeners and derivatives, and some siloxane substances.

You select which substance(s) that you are interested in, and then you can download the information in several different structures and formats (.csv, JSON, and xml).

The website is at https://apps.iowasuperfund.uiowa.edu/pcb-ids/

What's included?

Identifiers for the 209 PCB congeners and some of their derivatives, plus 6 siloxanes, compiled from PubChem, the EPA CompTox Chemicals Dashboard, and substance lists from Xueshu Li and Hans-Joachim Lehmler of the ISRP Synthesis Core.

Which identifiers?

One or more of the following are provided for each substance:

- Canonical SMILES
- CAS Registry Number
- DSSTox Substance ID
- InChI Key
- IUPAC Name
- PubChem CID

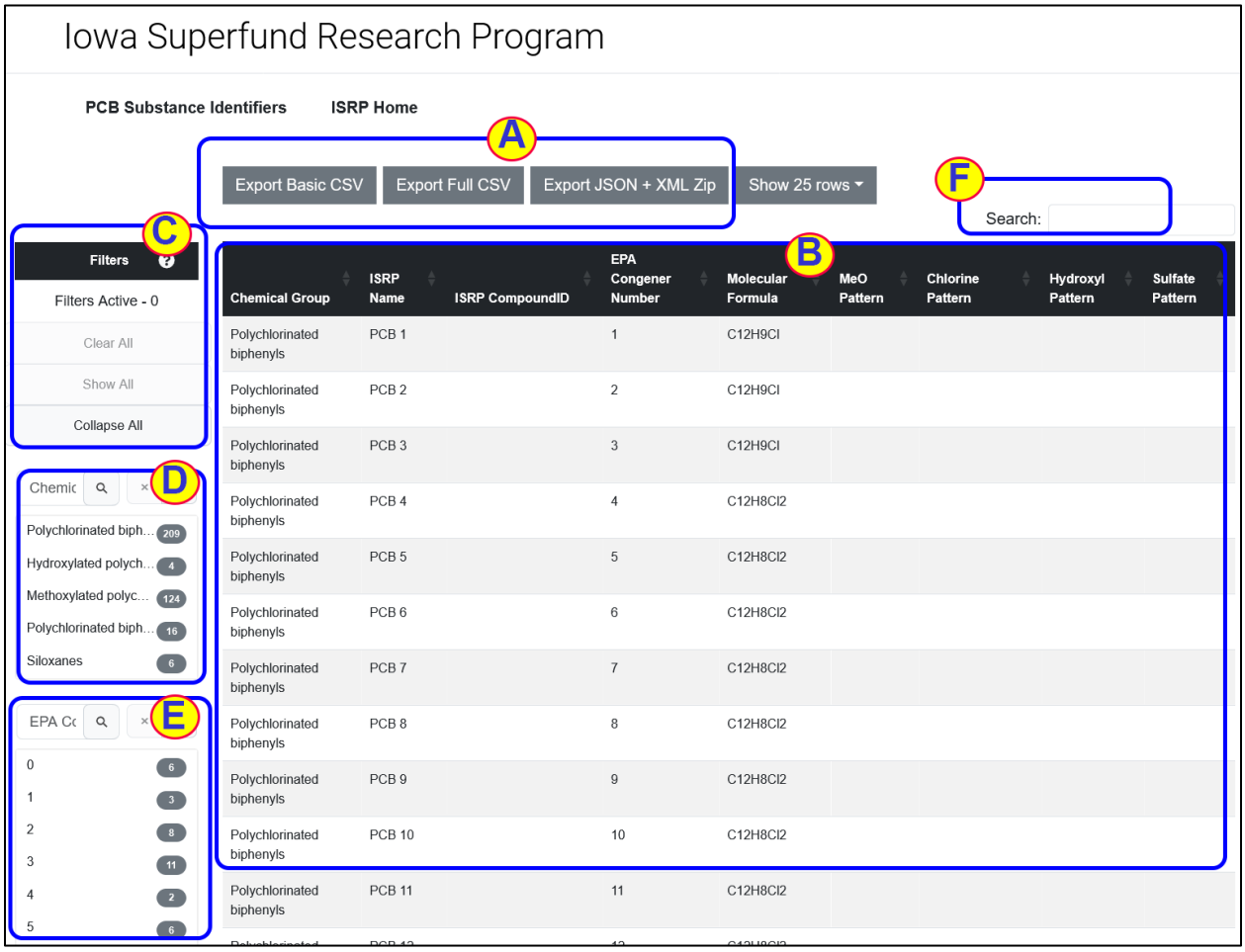
The web application was developed by Ted Fitzgerald, Lead Developer, CIO Office.

Contact: UI Data Services Librarian, brian-westra@uiowa.edu

I. Home Page Overview

When you open the web page, you'll see a table showing some of the PCB names, and several options for browsing, filtering, and exporting the information.

* Instructions below refer to the parts of the web page pictured below by letter.



A: Export options

After you have selected the record(s) you are interested in, use these options to export the information into files for your publication, and to include with your data deposit in IRO.

B. The main table of information

a) **Sort** by clicking on one of the column headings.
b) You can **select** one or more rows in this view and then export them.
c) The table immediately updates to display the substances matching any selected filters for chemical groups (D), and/or congener numbers (E).

C. Filters

This tells you how many filters are being applied to the table and is automatically updated when you change filter settings. The main table is immediately updated to display matching results.

D. Chemical group

Filter the displayed substances by chemical group (PCB congeners, derivatives, and some siloxanes).

- Substances listed are limited to those for which at least one computed identifier is available (InChI, InChIKey, SMILES). If a substance that you need is not in the table, contact us.

E. Congener numbers:

Another way to filter is by selecting one or more congeners (includes derivative(s) associated with those congeners).

F. Search

Search only finds exact matches to the string entered, including punctuation and spaces.

II. Select all of a group of substances

1) If you want **all of** the PCB congeners, or **all** of one or more types of derivatives, or **all** of the Siloxanes, select the **Chemical Group** (D).
2) The **Filters** (C) and the **table** (B) will immediately update to display the matching selections.
3) Once you have the **Chemical Group** you want, you can **Export** the tables (A). **Export Instructions below.**

If you want to start over, **Clear** your selection in the **Filters** window (C).

III. Select individual compounds or create a group of substances

There are several ways to select individual substances:

1) Choose the Chemical Group (D), then:
   - For **PCB**s, select the **Congener number**(s) corresponding to the PCB or derivatives (E)
     - or scroll through the table (B) and select individual substances.

- For **Siloxanes**, select the Chemical Group, then select individual substances in the table (B).

2) Go straight to the main table (B) and browse for a substance.
3) Search for a substance (F).
    - Search **only finds exact matches**, including spaces and punctuation, so it may be better to scroll or browse.

IV. Export the identifier files

Export these three files: Basic CSV, Full CSV, and JSON+XML.Zip.

1) Add the Basic csv file to your dataset deposit, and list and describe it in the README.txt file.
    - See the IRO data deposit guide for more details or contact the data librarian.
2) Send the Full CSV file and the JSON+XML ZIP file to the ISRP data curator, noting which dataset they are for.