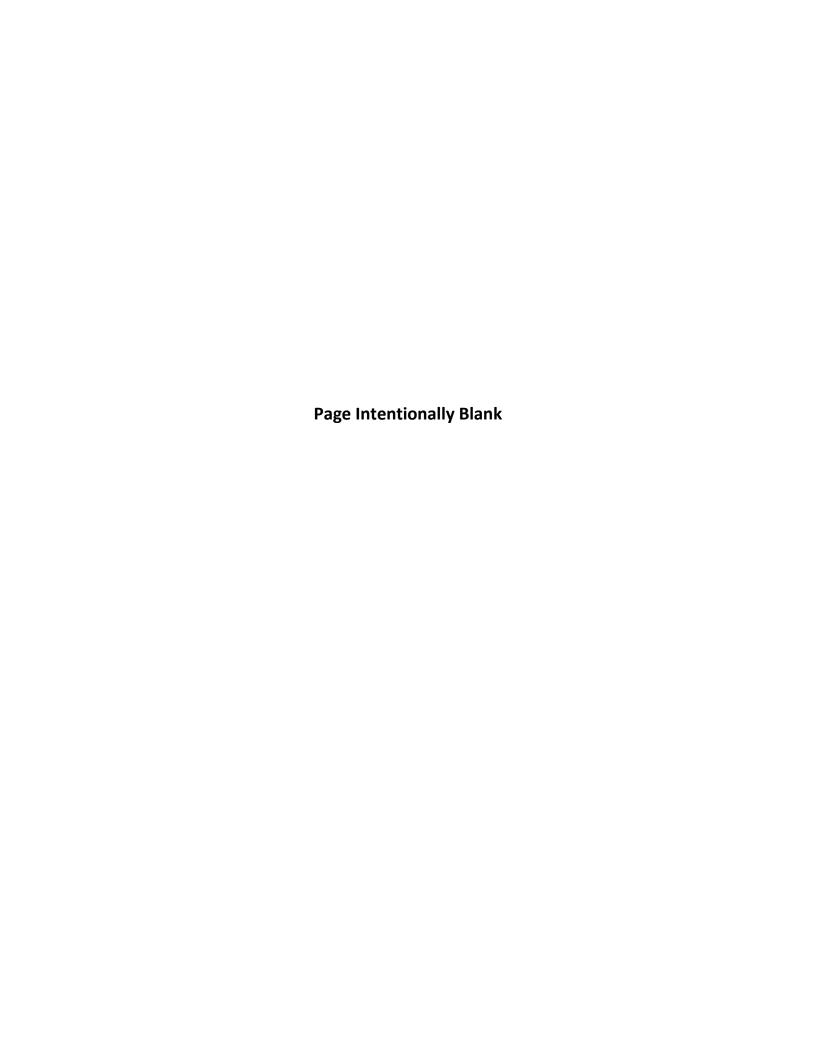


# Substance Registry Services End User Guide for Substance Search

Data Management Services Division EPA / Office of Environmental Information

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## 1 Introduction

This document serves as a guide for the search function of the Substance Registry Services (SRS) for the end user. The SRS is the Environmental Protection Agency's (EPA) central system for information about substances that are tracked or regulated by EPA or other sources. It is the authoritative resource for basic information about chemicals, biological organisms, and other substances of interest to EPA and its federal, state and tribal partners. The system provides a common basis for identification of, and information about, chemicals, biological organisms, physical properties, and various miscellaneous objects. This document provides instructions for the information scientists, subject matter experts and managers who wish to access substance data from SRS.

All functions are accessible from the the SRS homepage (www.epa.gov/srs).

## 2 Search by Substance Name or Identifier

The basic SRS search supports searching by Substance Name or identifier. Substance Names are chemical or biological names, the EPA Registry Name or other synonym. Substance Identifiers include Chemical Abstract Service (CAS) Numbers, Taxonomic Serial Numbers (TSN) <a href="http://www.itis.gov">http://www.itis.gov</a>, EPA Identifiers, Internal Tracking Numbers, or other Alternate Identifiers.

#### 2.1 Basic Search

The basic substance search has these steps:

- 1. Enter a Substance Name and select the appropriate search type represented by the radial buttons: Contains, Begins With, Exact Match. Contains is the default.
- 2. Or, enter a Substance Identifier.
- 3. Click Search.

Fig. 1 shows the results for a search on the word "acetone"

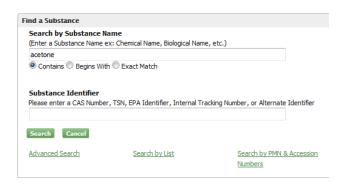


Fig. 1 SRS Find a Substance Search Box

The results are displayed along with the options to refine your search further using keywords or to export all or selected results (see Fig. 2).



Fig. 2 Substance Search Results

## 2.2 Filter by Keyword

A keyword is a single string of characters that occurs in the Substance Name. To filter by a keyword, enter the term in the box and press filter. In Figure 3, the keyword "cyclohexane" is added to filter results to include only those substances with that term. The page refreshes and only those substances with that keyword are displayed. Click on "Return to Results" to return to the unfiltered results.

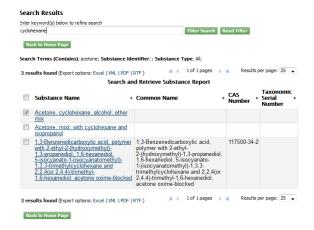


Fig. 3 Filtered Search Results

## 2.3 Export Search Results

One or more results can be exported in Excel, XML, PDF or RTF (Rich Text Format). Select all results by checking the box to the left of "Substance Name", or select one or more specific substance records for export by clicking on one or more check boxes to the left of the name in the Substance Name column (see Fig. 3). To deselect all, click the box to the left of the column heading labeled Substance Name.

#### 2.4 View Metadata and Substance Details

To view standard metadata and associated list information, click on the name itself. The standard metadata returned for these substances includes: Systematic Name, Common Name, CAS Number, and Taxonomic Serial Number (for biological substances only).

To view the substance details, click the selected Substance Name link. The Substance Details page provides additional information or links to pages about health information, chemical structure, and relevant EPA regulations and programs.

For example, clicking on the substance "Acetone, cyclohexane, alcohol and ether mix" accesses the Substance Details page shown in Figs. 4, 5 and 6.



Fig. 4 Top Part of Substance Details Page



Fig. 5 Middle Part of Substance Details Page



Fig. 6 Bottom Part of Substance Details Page

To see more metadata, click the Show More Metadata link (see Fig. 4). The results of the metadata expansion are shown in the right panel in Fig. 7.

## Acetone, cyclohexane, alcohol, ether mix

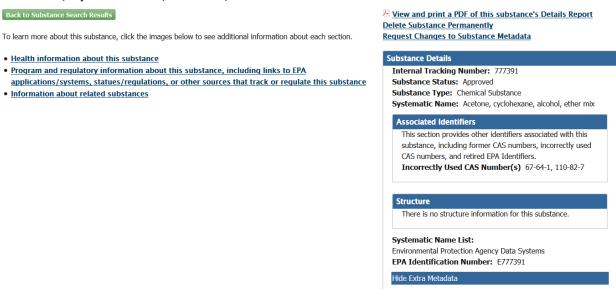


Fig. 7 Metadata Expansion

There are also a variety of output options for the Substance Details Report including a view or print of a PDF version.

#### **3** Advanced Search

The advanced search provides Boolean search capability and is only available on the public interface. This can be accessed from the main page by clicking the Advanced Search link, below the Search by Substance box (see Fig. 8).

#### **Chemical and Substance Resources**

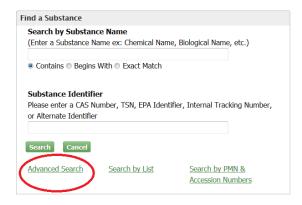


Fig. 8 Advanced Search Link

Fig. 9 shows the Advanced Search screen with the Criteria Type drop down list open. Advanced Search allows you to specifically search for any of the following criteria: Synonym, Substance Type, List Name, CAS Number, TSN, EPA Identification Number, Alternate Identifier, Classification, Characteristic or

Reason for regulation. The search options will depend on the criteria type selected; some criteria such as type and characteristic have drop down pick lists, while others such as Synonym are free form entry fields. For these criteria, radial buttons allow results to be filtered by Contains, Begins With, Exact Match, or a case sensitive Exact Match. The default is Contains. It also allows for return of records by Substance With Components, Substance Without Components or Both. The default is Both.

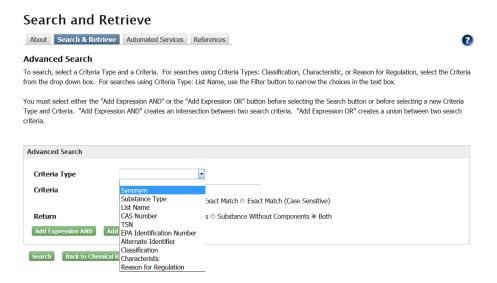


Fig. 9 Advanced Search

Figure 10 shows how to combine criteria with Boolean and/or operators to develop more precise search strategies. In this case a search for synonyms containing "Acetone" is being combined with another criteria using the "Add Expression AND" button.

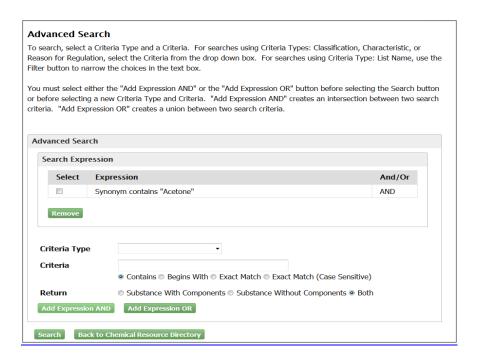


Fig. 10 Advanced Search Expression

#### To use the Advanced Search feature

- 1. Select Criteria Type.
- 2. Select the Criteria from the pick list.
- 3. If displayed for the selected criteria type, select one of the four Criteria Radial Buttons: Contains; Begins With; Exact Match; Exact Match (Case Sensitive). Contains is the default.
- 4. If displayed for the selected criteria type, select one of the three Components Radial Buttons: Substances with Components; Substances without Components; Both. Both is the default.
- 5. Select the Add Expression ADD or the Add Expression OR button to create a more complex Boolean search and enter the remaining criteria.
- 6. Press Search

The results are displayed as shown in Fig. 11.

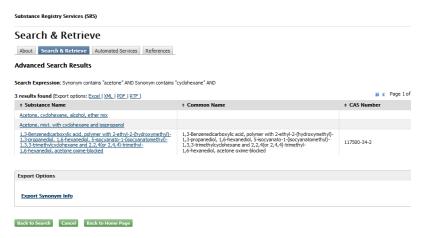


Fig. 11 Advanced Search Results

## 4 Search by Substance List and List Record Retrieval

Using the basic and advanced search you can find which lists are associated with a certain record. However, you may be more concerned with what records are included on or associated with certain individual lists. Perhaps you wish to perform a substance search limited to a certain list. You may also want to obtain a complete list of records contained within a given list. Using certain functions within the SRS search, it is possible to retrieve one, some or all records for a selected list, and view them. Use the following instructions to see the different methods possible.

## 4.1 Search by Substance List

The Search by List function allows you to limit the scope of your search to just one list. It works just like the basic search, but only applies to one specific list of your choice. The first step is to click on the Search by list link on the SRS home page as seen in Fig 12.

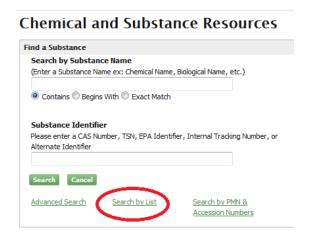


Fig. 12 Search by List Link

This page limits the subsequent searches to a specific list. For example, to check the "Great Lakes Environmental Database" for "Aluminum", scroll down the menu to select the Great Lakes list as seen in Fig 13. In addition to scrolling the list, the filter option can be used to search for a specific word in the

list name. This will narrow the list names to only those containing that word, and may make it easier to find the appropriate list.

## Search and Retrieve About Search & Retrieve Automated Services References Search by List 'o search, you must select a list name. Choose additional search criteria to narrow your selection. Then press the Search button. Please select a list from the menu below. This may be an EPA application/system, statute/regulation, ad hoc, or other external list that contains substance data To select a list, enter a list name (or acronym), then click "Filter" to narrow the number of lists displayed below. 6 Filter After clicking "Filter," select the list you would like to search on by clicking it. FDA (14290) - Food and Drug Administration Substance Registry FIFRA-Inerts (2198) - Inert Ingredients in Pesticide Products GCES (32047) - Green Chemistry Expert System GLFMP (50) - Great Lakes Fish Monitoring Program GRTS (61) - Section 319 Grants Reporting and Tracking System Fig. 13 List scroll down menu 1 Filter After cicking Tifter," select the list you would like to search on by cicking it. FDA (14200) - Food and Drug Administration Substance Registry FIFRA-Inters (2198) - Inter Impedents in Pestidie Products GCES (2047) - Green Chemistry Expert System (FIFRA-Inters (2004) - Green Chemistry Expert System (FIFRA-Inters GLENDA (457) "Great Lakes Environmental Database GLFMP (50) - Great Lakes Fish Monitoring Program GRTS (61) - Section 319 Grants Reporting and Tracking System Please enter a CAS Name, Biological Name, EPA Registry Name or other Synonyn Aluminum O Contains Degins With Exact Match Please enter a CAS Number, TSN, or EPA Identifie Return Substance With Components Substance Without Components Both

Fig. 14 Search by List Synonym search

Search Cancel Back to Chemical Resource Directory

ate Identifier, please select an Alternate Identifer Context.

Press and hold the "CTRL' key while left-clicking to select or deselect multiple characters benecommatter degradant degradant dre industrial chemical "

Current Substances Only Pending Substances Only Both Pending and Current Substances

The next step is to perform a search for a record as described in Section 2. This will display results for your search, but will only return results from your specific list as seen in Fig. 15.



Fig. 15 Search by List results for Aluminium

A search on the same list using a broader term like "Aroclor" retrieves multiple substance results (see Fig. 16).

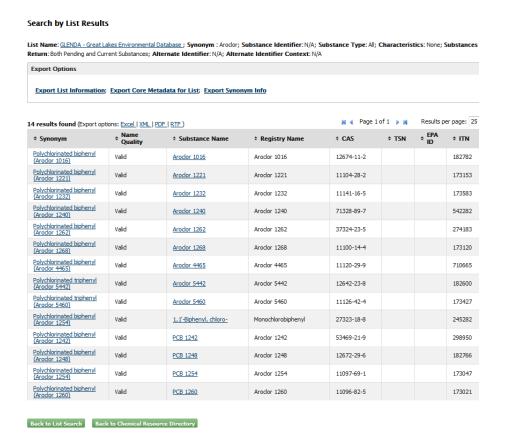


Fig.16 Results for Aroclor in a search of the GLENDA list

As described in Section 2, you can select the specific record to view the record's data. The metadata can be exported for these results by using the links at the top of the results. Select a link for Excel, XML, PDF or RTF formats as seen in Fig.17.

#### Search by List Results

List Name: GLENDA - Great Lakes Environmental Database; Synonym: Arodor; Substance Identifier: N/A; Substance Type: All; Characteristics: None; Substances Return: Both Pending and Current Substances; Alternate Identifier: N/A; Alternate Identifier Context: N/A **Export Options** Export List Information; Export Core Metadata for List; Export Synonym Info N A Page 1 of 1 N Results per page: 25 results found (Export options: Excel | XML | PDF | RTF.) Name \* Registry Name + CAS **⇒ TSN** + ITN Polychlorinated biphenyl (Arodor 1016) Arodor 1016 Arodor 1016 12674-11-2 182782 Polychlorinated biphenyl (Arodor 1221) Arodor 1221 Arodor 1221 173153 Polychlorinated biphenyl Arodor 1232 Arodor 1232 11141-16-5 173583

Fig. 17 Export Search by list results

#### **4.2 Find All Records** for a Substance List

To find all records associated with a particular list, return to the SRS home page and then select the Search by List page. Select the list following the instructions in 4.1, but do not enter anything in the search box. A blank search returns all the records for that list. Fig. 18 shows results from a blank search of "Great Lakes Environmental Database."

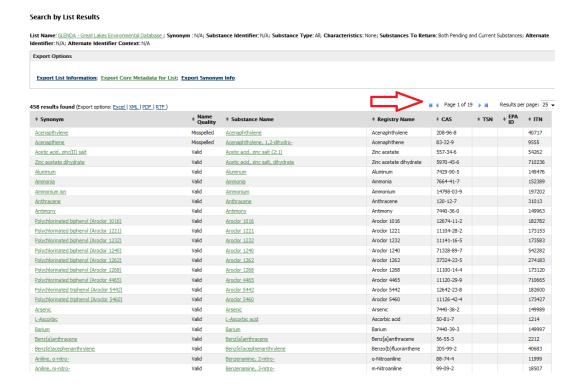


Fig. 18 All records contained within a list

The initial display is limited to the first 25 results for this list. Use the page slider at the top to change the page, or the Results per page drop down menu to alter the number of records in a display.

Note: If you try to view the records for a list that exceeds 1500 records you will get the following message:

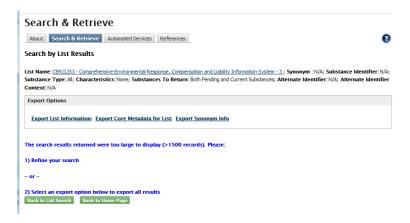


Fig. 19. Search results too large to display

The complete list of records can still be obtained by downloading a .CSV file containing a table with all the records for this list. To obtain this table, use the "Export Core Metadata for List" option in the Export Options box on the search results page (see Fig. 20). This will download a file that can be opened in Excel, including the following fields for each record: Internal Tracking Number, CAS#, EPA ID#, TSN#, Substance Name, Substance Name List, Registry Name, Registry Name List, Synonym Effective Date, Synonym End Date, Definition, Comments, Retired CAS#s, Incorrect CAS#s, Structural Notation Type, Structural Notation, and Related Links. See Fig. 21.

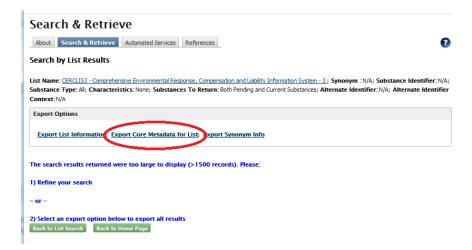


Fig. 20 Export Core Metadata

Internal T	CAS#	EPA ID#	TSN#	Substance Name	Substance	Name Lis	t Registry N	Registry N	Synonym	Synonym	Definition	Comment	Retired C	Incorrect	Structural	Structural	Related Links
16410	95807			1,3-Benzenediami	Chemical A	bstracts I	2,4-Tolue	Chemical	Identificat	ion			85898880,	25376458	SMILES	Nc1c(ccc(c	[Name: Hazard
17002189	72333			19-Norpregna-1,3,	Chemical A	bstracts I	Mestrano	Chemical	Identificat	ion					SMILES	COc1ccc20	[Name: Chemi
5538	75354			Ethene, 1,1-dichlo	Chemical A	bstracts I	1,1-Dichlo	Chemical	Identificat	ion					SMILES	C(=C)(CI)C	[Name: Hazard
121491	4098719			Cyclohexane, 5-is	Chemical A	bstracts I	Isophoron	Chemical	Identificat	ion			26602937,	158750302	SMILES	O=C=NCC:	[Name: NIOSH
221978	22481487			Radon, isotope of	Chemical A	bstracts I	Radon-22	Chemical	Identificat	ion			14835031				[Name: Lund l
106427	2703131			Phosphonothioic a	Chemical A	bstracts I	O-Ethyl O	Chemical	Identificat	ion			1942569				[Name: NJ RTk
41020	287923			Cyclopentane	Chemical A	bstracts I	Cyclopent	Chemical	Identificat	ion					SMILES	C1CCCC1	[Name: OSHA
154542	7783188			Thiosulfuric acid (	Chemical A	bstracts I	Ammoniu	Chemical	Identificat	ion			15824314		SMILES	[NH4+].[S-	[Name: Chemi

Fig. 21 Exported Core Metadata

The synonyms for each of the records can be viewed by using the Export Synonym Info function (Fig. 22). This function provides a list of all Substance Names and their respective Synonyms. Clicking on this link initiates a download of a .CSV file that can be opened in Excel. The table includes all the records for this list, as well as associated metadata (Fig. 23). The associated fields for each record are Substance Name, Internal Tracking Number, CAS or TSN #, Registry Name, Synonym Name, Synonym Start and End dates, Lists and Components of another Substance.



Fig. 22. Export Synonym info.

Internal Tracking Number	CAS#	EPA ID#	TSN #	Substance Name	Registry Name	Synonym Name	Synonym	Synonym	Lists	Compon
17000993	6055-19-2			2H-1,3,2-Oxazaph	Cyclophospham	Cyclophosphamic	de (hydrate	ed)	CERCLIS3	N
76661	1024-57-3			2,5-Methano-2H-i	Heptachlor epox	Heptachlor epoxi	de		ERNS, ECOTOX, SA	ΔY
159848	8032-32-4			Ligroine	Ligroine	Varish Makers &	Painters na	phtha	CERCLIS3	Υ
76745	1031-47-6			Phosphonic diam	Triamiphos	Triamiphos			EPCRA 302, FDA, I	Y
303834	55283-68-	6		Benzenamine, N-	Ethalfluralin	Ethalfluralin			ChemIDStd, Merc	ΙY
40758	225-51-4			Benz[c]acridine	Benz[c]acridine	Benz[c]acridine			RCRA Appendix V	N
75101	950-10-7			Phosphoramidic a	Mephosfolan	Mephosfolan			ChemIDStd, FDA,	Υ
150078	7440-48-4			Cobalt	Cobalt	Cobalt			WQX, CWA 304B,	(Y
2113	56-35-9			Distannoxane, 1,1	Bis(tributyltin)	Bis(tributylin) ox	ide		EPCRA 313, CERCI	N

Fig. 23 Exported Synonym info.

## 5 PMN & Accession Number Search

The SRS can also be searched using alternate Identifiers, such as Premanufacture Notice (PMN) & Accession Numbers using the respective searches in Fig. 24. These searches are useful for finding records associated with the TSCA or Toxic Substance Control Act lists.

#### **Chemical and Substance Resources** Find a Substance Search by Substance Name (Enter a Substance Name ex: Chemical Name, Biological Name, etc.) Ocontains Begins With Exact Match Substance Identifier Please enter a CAS Number, TSN, EPA Identifier, Internal Tracking Number, or Alternate Identifier Search Cancel Search by PMN & Accession Numbers Advanced Search Search by List Health Resources New Jersey RTK Fact Sheets ToxFAOs Enforcement and Compliance History Online (ECHO/IDEA) NIOSH Occupational Health Guidelines for Chemical Hazards MyEnvironment More Health Information Resources More Popular Resources Integrated Risk Information System (IRIS) Lead Renovation DSSTox Pesticides Registration ChemView TRI Reporting More Scientific Information Resources More Business and Industry Information Resources

Fig 24. Search by PMN & Accession Numbers

## **5.1 Search by Premanufacture Notice (PMNs)**

Section 5 of the TSCA requires anyone who plans to produce or import a new chemical substance to provide the EPA with a Premanufacture Notice or PMN at least 90 days prior to production. These identifiers are contained within the TSCA lists in SRS as alternate identifiers and can be searched to find related records. Click on the Search by PMN & Accession Numbers search in Fig 24. Then in Fig 25. enter the PMN identifier in the "identifier" search box. Exclude any dashes in your PMN identifier so that it appears as a single string (e.g., "P810312"). Make sure the PMN box is checked. Click search to obtain record results as seen in Fig. 26. Both the Accession Number and the Generic Name for the PMN are displayed. The whole record can then be found by using the basic search (Section 2) on the Generic Name.

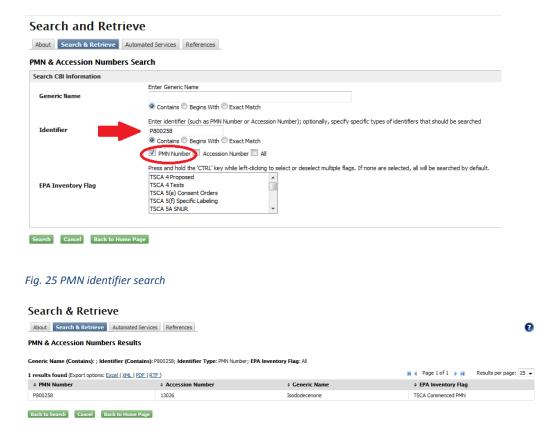


Fig. 26 PMN identifier results.

## **5.2 Search by Accession Number**

Chemicals in the TSCA lists may also be identified by an Accession Number. Click on the Search by PMN & Accession Numbers search in Fig. 24. Then in Fig. 27, enter the Accession Number in the "identifier" search box. Make sure the Accession Number box is checked. Click search to obtain results as shown in Fig. 28. Both the PMN and the Generic Name are displayed. Use a basic search on the Generic Name (Section 2) to obtain full record information.

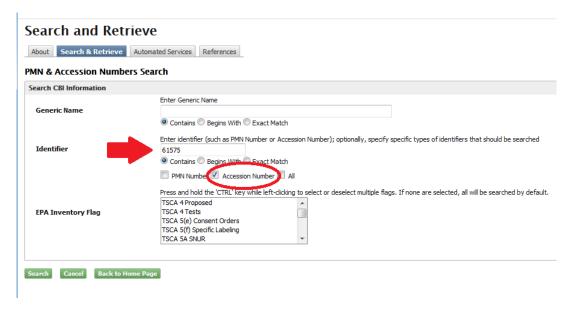


Fig. 27 Accession Number Search



Fig. 28 Accession Number Results

## 5.3 Search by Generic Name

If you happen to know the Generic Name of your TSCA list substance, but want to find either the PMN or Accession Number, click on the Search by PMN & Accession Numbers search in Fig 24. Then as shown in Fig. 29, enter the Generic Name in the "Generic Name" search box. Click search to obtain results as shown in Fig. 30. Both the PMN and Accession Number are displayed for the Generic Name.

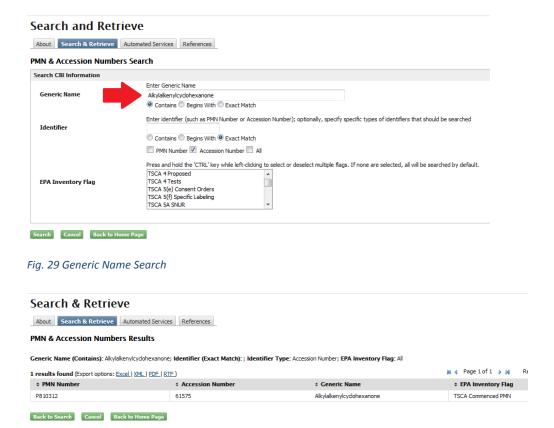


Fig. 30 Generic Name Search results