iResearch™ System Fast Start Overview

This document is designed to assist you by introducing key features of the iResearch System. The iResearch System is an Internet application that provides you access to ChemNavigator's iResearch Library database of commercial screening compounds. The iResearch Library database can also be licensed on disk. The iResearch Library is updated frequently to reflect the most recent information available from suppliers. A single search of the database using the iResearch System application (2D substructure and/or similarity search) allows you to search offerings from suppliers worldwide.

This document covers the following topics to help you search, review and manage your data in the iResearch System:

- **Conducting a Search**
- **Reviewing Search Results**
- **Sourcing and Procuring Compounds**
- **Managing Project Results**

Conducting a Search

This section explains how to use the iResearch System to define your Preferences by setting your Database, Chemistry, and Business preferences. You will also learn how to conduct a search of the iResearch Library and our Content databases. Log into your iResearch System account before following the suggestions below.

Objective:

- Defining Preferences
- Setting Database Preferences
- Setting Chemistry Preferences
- Setting Business Preferences
- Conducting a Search
- Sample vs. Content Records
- Allowing Sample and Content Duplicates

Defining your Preferences

Your Preferences are initially defined by the Database, Chemistry, and Business Preferences that you select, which define the commercial compound (Sample) records and information (Content) records that will be searched based on your structure query. To access these preferences, click on **Preferences** in the left side navigation bar.

Setting the Database Preferences

Click on **Database Prefs**. All searchable content available to you will be listed and divided into 3 major categories:

1. **iResearch Library:** select which sample collections within the library that you wish to search (see Appendix A for descriptions of the content of each collection);
2. **Content Databases:** select from databases providing additional data related to chemical structures.

Setting the Chemistry Preferences

Click on **Chemistry Prefs**. You can choose preset drug-like chemistry preferences from the drop-down menu, or your can make your own selections under Molecular Properties, Pharmacophore Elements, and Undesirable Chemical Groups. These preferences allow you to define drug-like and other criteria that are relevant to a particular search.

Setting the Business Preferences

Click on **Business Prefs**. The Business Prefs allow you to define sample requirements such as Minimum Purity and Shipping Window. Setting specific preferences will exclude any samples that do not meet these requirements prior to the search. For example, samples that should deliver within 30 days and that have 90% or greater purity. ChemNavigator provides information provided by the supplier and allows you to determine which business preferences are critical to your project.

Conducting a Search

Click on the "Search" link on the left-hand navigation bar. You will see a list of search options including the standard **Structure Search**, the optional **ISIS Paste**, **List Entry**, **Keyword Search**, and **SDF Structure Match** options.

Structure Search

You may select **Structure Search** to have access to use of the following search options: The **JME Simple Sketcher** (provided by Novartis), **ChemDraw4** or **ChemDraw7 plug-ins** (after download and installation), or our **Structure Notation Entry** tool which allows you to enter **an SDF, SLN, or SMILES** character string. When using the Structure Search options, you can control the following settings:

- Type of search you conduct - similarity, substructure, or both
- Desired similarity percentage (search radius)
- Whether to allow or prevent structural duplicates from being displayed in your results
- Whether to allow substitution at all hydrogen atoms
- Whether to have the JME Simple Sketcher fill all unspecified valances with hydrogen's (valences are not automatically filled when using this sketcher)
- The maximum number of hits at which the search terminates
- Name of your Results List

For more detail on using the JME Simple Sketcher, ChemDraw plug-in, or Structure Notation Entry, click on the **How to use...** below the sketcher window.

ISIS Paste

You can select the ISIS Paste option if you would like to paste in an existing sketch from ISIS Draw/Base/Host. Please refer to the link in ISIS Paste window to properly configure your ISIS application before copying and pasting your structure. When using the ISIS Paste option, you can control the search settings after pasting in a structure.

List Entry

If you have a list of CNC_ID values (ChemNavigator sample ID values) or a list of STRUCTURE_ID values (ChemNavigator structure ID values) from a prior search or from the iResearch Library database on DVD, you can paste up to 500 into this window to lookup the samples.

Keyword Search

The Keyword Search option allows for searches using chemical name and/or CAS Number. Note that for most novel screening compounds, the suppliers have not assigned CAS numbers.

SDF Structure Match

This tool allows you to upload an SDfile of structures. The iResearch System will normalize your structure records to match the iResearch Library database rules and will look for exact, active matches in the iResearch Library.

Sample versus Content Records

There are two types of structure records that are represented while viewing a Result List:
A **Sample Record** represents an actual physical sample that is available for procurement through suppliers contributing to the iResearch Library.
A **Content Record** represents a structure linked to related information known about that structure, for example, whether the structure is an FDA-approved ingredient. Content records are found in the non-supplier databases accessible through the iResearch System, such as our FDA Orange Book Active Ingredients databases. (Note: Structures in content records may not available commercially – if a commercial option is available, it will be listed separately as a Sample record).

Allowing Structure Duplicates

Sample Records: If Sample Duplicates are allowed, you will see a Sample Record for each supplier that provides the structure. If the duplicates are NOT allowed, the structure will appear once, and the Sample Detail button can be used to see alternate sources for the same structure.

Content Records*:* If Content Duplicates are allowed, you will see all occurrences of the structure within any of the Content Databases searched. If duplicates are NOT allowed, you will only see the first occurrence found from our Content Databases, additional matches will not be displayed. We recommend that you Allow Content Duplicates to see all content matches.

Once you have chosen the settings that are relevant to this search, enter your chemical structure and click on the **Search** button. After the search has completed, you will see a summary of search-result statistics indicating how much of the database was searched, why certain compounds were excluded, and the number of compounds that matched your search query. Click on **View Results** to see the structures that matched your query. If no compound records were found, either change the preferences you set (*Database, Chemistry or Business Prefs)*, or modify the structure query and settings you entered.

Searching and Search Credits

Named-user subscriptions to the iResearch System provide unlimited searches. Your 7-Day Evaluation account, though, has a limited number of Search Credits. Once these have been used, you will need to contact your representative or ChemNavigator Support (support@chemnavigator.com) before trying to view additional search results.

Reviewing Search Results

This section explains how to view, sort and organize your search results (Result Lists). To help illustrate our explanation, we will have you use a list that you have already created from the **Conducting a Search** section (*page 1-3 of this document)*.

Objectives:

- Viewing and organizing search results
- Changing the display mode
- Selecting Samples
- Filtering the results list
- Sorting the results list
- Structure controls
- Launching a search from a result list
- Record Detail Report to view all sources for a sample
- Zooming and Downloading chemical structures

Viewing and Sorting Search Results

Note*: You must conduct at least 1 search and save the results prior to this section*.
Login and click on the **Project Results** link in the left side navigation bar. Select **Recall List** from the submenu and select a list to view. You will be taken to the Result Browser page and will be able to view the search results. Search results are initially presented in order of relevance to the query - substructure matches first, then by similarity. For substructure matches, the substructure will be highlighted in each structure. You can use the Display Controls at the top of the page to sort and view your results in a variety of ways. Each structure record is shown with related data such as supplier, molecular weight, cLogP, purity, availability, and shipping times. Sample Records are indicated with a tan border on the left, and Content Records are indicated with a red border on the left.

Changing the Display Modes

Figure 1
These buttons allow you to change your display mode.

At the top of the Result Browser you will find 4 buttons grouped together (*Fig. 1)* that allow you to control how you view your search results. The first 2 buttons from the left allow you to control how much information is displayed for each structure by switching between Detail and Tiled Views. Detail View provides all accompanying sample data. Tiled View displays only chemical structures with ID numbers (sample detail can then be viewed using the View Record Detail button – see Structure Detail Report below). The third and fourth buttons from the left allow you to view the samples in Page-by-Page (non-clustered) or Clustered

Mode. Page-by-Page mode displays 20 samples per page based on your selection from the "Sort Sample By" menu. Cluster View identifies and displays the 20 most diverse structures in your search results. The remaining structures are categorized under each of these clusters and can be viewed by clicking on the **Browse Cluster** button.

Selecting Samples

To select samples in your list, simply click the check box next to the record's CNC ID. After you have made your selections click the Save List* button (*left button in Fig. 2*). You may also select all of the samples in your list by clicking the Select ALL button (*center button in Fig. 2*). Finally, you may de-select all samples in your list by clicking the De-Select ALL button (*right button in Fig. 2)*

Figure 2

**Note: If you select samples individually, you must click the Save List button in order to update your selections for the list. The Select ALL and De-Select ALL buttons update automatically*

Filtering by Collection

The "Filter by Collection" menu allows you to view samples from a specific collection within the iResearch System Library or a specific Content Database by selecting the database from the menu.

Filer by Status

Results can be filtered to show ALL, Selected and Un-selected records, to allow you to quickly examine your selections.

Sorting Your Results

Results can be sorted in a variety of ways by using the selections under the "Sort Sample By" menu including Similarity to Query, Supplier Name, and Shipping Window.

Launching a Search from a Structure Record

A **List Search** button is located under each chemical structure. Clicking on this button will place a copy of the structure in the Search window and allow you to conduct a search of the structure.

Structure Detail Report

The **View Record Details** button located under the structure will enable a printable pop-up window that provides all available information on a given chemical structure, including alternate supplier sources. When Sample Duplicates have not been displayed, this window allows you to see all other sources for the structure. It also provides access to all sample information when you are using Tiled View.

Zooming and Downloading Chemical Structures

To zoom a structure, click on the actual structure, and a larger sketch will appear. If you click on this pop-up window, you may obtain an even larger sketch of the compound.

The **SMILES**, **SLN**, and **SDF** buttons located under the structure will generate a pop-up window containing a text string for each chemical structure. As an additional feature, we offer an SDfile (SLN or SMILES) download for an entire Result List. This download to file option is not active for a 7-Day Evaluation Account. If you would like access to this feature during your evaluation, please contact your sales representative.

Result Browser Help

Detailed help is available online, describing all the buttons and features of your Result List. Please review this page by clicking the question mark button in the upper left side of the Result Browser.

Sourcing and Procuring Compounds

Note: *You must conduct at least 1 search and save the results prior to this section*.
This section provides an overview of sourcing of samples, direct ordering of samples using the Sourcing Report, and the option for customers to use ChemNavigator's Procurement Service. Login to your account, click on the **Project Results** link on the left-hand navigation bar. Click **Recall List** from the submenu, and then click one of your Result Lists.

Ordering Direct using the Sourcing Report

As an iResearch System subscriber, you can select to order compounds of interest directly from the supplier or use ChemNavigator's Chemistry Procurement Service. When you wish to place an order directly with the supplier, you can use the Sourcing Report to provide supplier contact information and to show you all sources for each structure of interest.

To generate a Sourcing Report, you must first select the compounds of interest (*see "Selecting Samples" in the "Reviewing Search Results Section").* Once you have saved the records of interest, you can generate a Sourcing Report by clicking on the **Get Sourcing Report** button (*second button from the right at the top of the Result Browser*). The first window will allow you to select any suppliers that you wish to exclude from the report (*as well as to click on a supplier name to get contact information*). Select whether to create the report in HTML, text, or Excel format then click on the **Get Sourcing Report** button to generate the report. The Sourcing Report is not active for a 7-Day Evaluation Account. If you would like access to this option during your evaluation, please contact your sales representative.

ChemNavigator Chemistry Procurement Service

Purchasing a library of compounds from multiple international suppliers can be a time consuming and frustrating process. ChemNavigator has established relationships with many of the suppliers who provide the chemistry that is tracked within the iResearch Library. ChemNavigator can streamline the compound acquisition process by taking on the burden of sourcing and procuring the chemistry for clients.

To send a request for compounds to ChemNavigator through the iResearch System, first make sure that you have selected all the compounds that interest you. Click on the button with the dollar sign at the top of the Result Browser (fourth from the right). You will be taken to the Checkout page that allows you to select the Result List that you would like ChemNavigator to procure. Select the Result List and click on **Continue with Procurement**. At the Order Summary page you will be asked to select a sample quantity and provide any special instructions for your order and acquisition. Click on "Continue", and then confirm the contact information we have in our system, and click on **Complete Procurement Request**. Alternatively, you can download a list of CNC ID's for structures of interest and email them to support@chemnavigator.com.

To download a list of CNC ID's click on the "Structure Download" button (*located 3rd from the right at the top of the Result Browser window*). Select CNC IDs and either output to a file or to the browser window. To submit a request for these samples, simply email the list (or file) to support@chemnavigator.com, and our Support Group will contact you to confirm your order request.

After we receive your order request we will then contact each supplier to verify:

- Sample availability
- Sample price (for large purchases we can negotiate lower pricing)
- Delivery time

Depending on supplier response times, we will typically provide a price quote within 7 business days of receiving your request. The price quotation that we provide to you includes the cost of the sample, an estimate of shipping fees, and ChemNavigator's service fees. The order will not be placed until you approve the quotation. In addition to the sample cost, ChemNavigator charges shipping and a per-sample procurement fee. For more detailed information on our Procurement Service, please contact ChemNavigator.

Managing Project Results

Under the Project Results link, there are tools that allow you to manage the results from your searches, review your Result Lists that are ready for procurement and to review Result Lists that have been procured. The tools available are as follows:

- **Current List** - Redirects you to the last Result List that you created or reviewed.
- **Recall List –** Allows you to review all of the Result Lists you currently have active as well as Lists that were procured.
- **Delete List** - Allows you to delete Result Lists that you do not require
  Note: Procured/Ordered Lists may not be deleted and do not count against the List limit of your account.
- **List Logic -** List Logic allows you to perform logical operations involving lists, such as combining 2 lists, subtracting a subset of records or only selecting records that exist in both lists.

Your iResearch System Account

Thank you for your interest in the iResearch System. If you are already working with a ChemNavigator representative, your evaluation will remain active during your discussions. If you have not yet contacted your ChemNavigator representative, your account will be returned to Trial User status at the end of the evaluation period, and your Result Lists will expire one week later. If you are interested in institutional access or have questions or suggestions please e-mail support@chemnavigator.com or call us at +1-858-450-9740 x1341 and we will be happy to assist you.

CD/DVD Version of the iResearch Library

The iResearch Library is also available in structure data file format on CD/DVD for use within your internal system. Please contact us if you would like additional information on licensing the data on CD/DVD.

APPENDIX A: iResearch Library Collections

This is an overview of the iResearch Library Collection names that appear on the Database Prefs page. The Collection name can be used to select which sample groups to search, either by sample type or by commercial availability.

Within any collection, the Shipping Window field under the Business Prefs can be used to further refine the search and include only samples available within the desired timeframe (for example, 14 days or less, 30 days or less, etc.).

- **Drug-like Compounds**
  Sample records in the Drug-like Compounds collection consist of compounds identified by the supplier as small-molecule organics suitable for testing in a biological screening assay and are typically available in milligram quantities. Most have Shipping Windows of 60 days or less. Samples are typically in stock at the supplier or obtained by the supplier from an outside source.
  Availability[1] – High 80% to 90% (in low milligram quantities)

- **Natural Products**
  Sample records in the Natural Products collection consist of compounds identified by the supplier as natural compounds or their derivatives or analogs.
  Availability[1] – High 80% to 90% (in low milligram quantities)

- **Building Blocks**
  Sample records in the Building Blocks collection consist of compounds identified by the supplier as building block chemicals and are available through the supplier in milligram to multi-gram quantities.
  Availability[1] – High 80% to 95% (in gram level quantities)

- **Reagents and Fine Chemicals**
  Samples records in the Reagent and Fine Chemicals collection consist of compounds identified by the supplier as reagent grade or fine chemical materials available in gram to kilogram level quantities. These specialty chemicals are made available through ChemNavigator's growing network of specialty & fine chemical suppliers from around the world.
  Availability[1] – High 80% to 95% (in gram level quantities)

- **Made to Order Chemistry**
  This collection includes chemical structure records for products our Supplier Partners believe they can synthesize based upon their own experience and synthetic expertise. These chemical products may not have been synthesized before but are believed to be synthetically feasible by the supplier.
  When ordering through our Chemistry Procurement Service, reporting price and availability of custom synthesis chemistry will take additional time compared to other iResearch Library Collections.
  Availability[1] – Medium 60% to 75% (in milligram level quantities)

- **Virtual Custom Chemistry**
  The Virtual Chemistry Collection consists of primarily small-molecule organic compounds that are custom synthesized by the supplier upon receipt of a confirmed order. Price and availability are quoted upon request. Delivery times are typically more than 60 days. ChemNavigator has compiled this collection to provide access to a broader range of drug-like chemistry. If the original source is unable to provide the compound, ChemNavigator may be able to assist customers in locating an alternate source.
  When ordering through our Chemistry Procurement Service, reporting price and availability of custom synthesis chemistry will take additional time compared to other iResearch Library Collections.
  Availability[1] – Low - 50% to 60% (in custom ordered quantities)

- **Archived Compounds Collection**
  Sample records in the Archived Compounds collection consist of hard-to-find, drug-like compounds, which may not be readily available but could be interesting in pharmaceutical research. Delivery times are typically 90 days or longer. ChemNavigator has compiled this collection to provide access to structures for a broader range of drug-like chemistry. If the original source for a structure in the Archived Chemistry collection is unable to provide the compound, ChemNavigator may be able to assist customers in locating an alternate source. When ordering through our Chemistry Procurement Service, it may take longer to obtain price and availability information for these samples.
  Availability[1] – Very Low – 20% to 50%

1. Availability rating based upon using a current version of the iResearch Library and ordering sample sizes appropriate collection.

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