

SARvision|SM and CDD Vault

SARvision has functionality to connect with CDD Vault and import data stored in the Vault for easy Structure Activity Analysis (or Sequence Structure Analysis for SARvision-Biologics). The following steps show how to get access to your CDD Vault account and then pull data relevant to our analysis

1. Log in to the CDD Vault and got to **Settings**. Under **API Keys**, *Add a new key* to use with SARvision. Copy this key so that it can be pasted into SARvision in the next step. This key contains all the information to allow SARivision to have access to you CDD Vault database. Note that it can be deleted to remove access at a later date.

CDD.VAULT - Altoris Sandbox

Help · Log out

Explore Data ELN Import Data Reports **Settings** Mark Hansen

User Vault

Preferences

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Alerts

API Keys

Your API Keys

Create and copy a login key

Your new token named **Example Key** is below. Please copy it to a safe place - you won't be able to retrieve it later.

Note : you must protect this token as if it were a password.

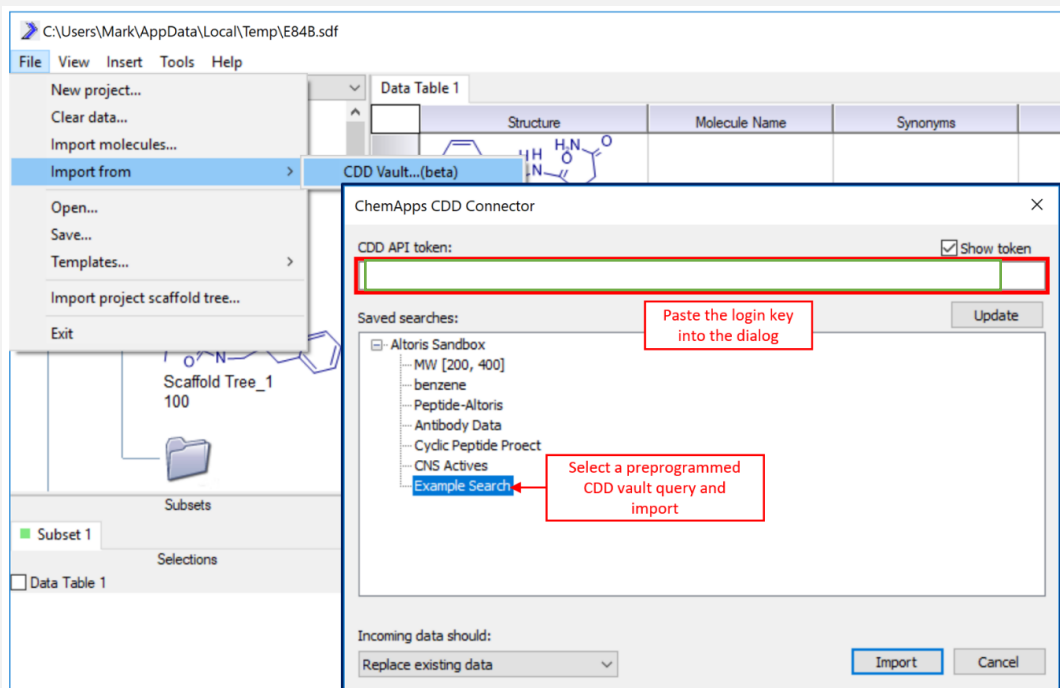
Name	Role	Token	
CDDapiKey	read only	[hidden]	Delete
Example Key	read only	[hidden]	Delete

+ Add a new key

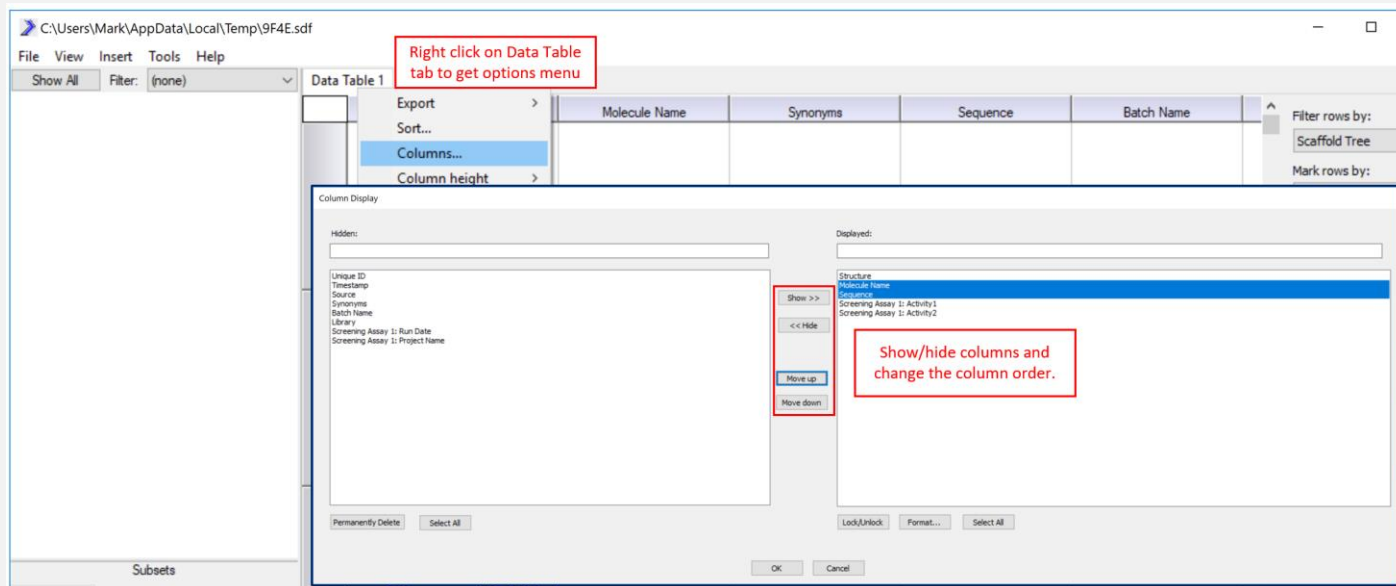
API-enabled Vaults

Altoris Sandbox

2. In SARvision|SM, under **File->Import from->CDD Vault...** paste the API token that you copied in step one into the correct box as shown. The Update button will reload the available saved queries in CDD Vault that you can access. If you do not have any, log onto CDD Vault and create some. In the ChemApps CDD Vault connector, select one of the queries and press the **Import** button.



3. Once you have loaded some data, right click on the Data Table tab and use the **Columns...** control to clean up the table and show only the relevant columns.



4. Right click on the Scaffold Tree workspace (upper left) to get a tree menu. Select **Identify scaffolds...** and use the default settings to generate relevant chemical cores or scaffolds that represent this particular dataset.

The screenshot shows the ChemApps interface with the Scaffold Tree workspace on the left. A right-click context menu is open over the Scaffold Tree, with 'Identify scaffolds...' selected. The 'Identify Scaffolds' dialog box is open, showing various options for tree building, scaffold display, and scaffold pruning. A red box highlights the 'Identify scaffolds...' option in the menu, and another red box highlights the 'Default settings' button in the dialog. A red arrow points from the 'Default settings' button to the Scaffold Tree workspace.

5. The user can edit any scaffold in the tree by right clicking on that scaffold and selecting **Edit scaffold...**. The user can also drag and drop scaffolds, delete scaffold and manually draw in scaffold using this menu.

The screenshot shows the ChemApps interface with the Scaffold Tree workspace on the left. A right-click context menu is open over a scaffold in the tree, with 'Edit scaffold...' selected. The 'ChemApps Molecule Editor' window is open, showing a chemical structure of a peptoid backbone. A red box highlights the 'Edit scaffold...' option in the menu, and another red box highlights the chemical structure in the editor window.

6. Additional view of the data can be added under **main menu->Insert**. In this example an R-Group table is added. To trigger rebuilding of the tables, double click on any scaffold. This will load the molecules that belong to that scaffold, reorient them relative to the scaffold and color code the molecules based on the scaffold.

The screenshot displays the SARVISION software interface. The main window shows a table with columns: R1, R2, R3, R4, Structure, Molecule Name, Synonyms, Sequence, and Batch Name. The table contains four rows of data, each representing a different molecule with its corresponding R-group structures. A Scaffold Tree on the left shows a selected scaffold (Scaffold Tree_1) with a red box around it and a text box stating "Double click the scaffold to trigger a view rebuild." The 'Insert' menu is open, showing the 'R-Group table' option highlighted, with a red box around it and a text box stating "Add a second view of the data: R-Group table." The interface also includes a 'Filter rows by:' dropdown set to 'Scaffold Tree', a 'Molecule scale:' dropdown set to '75%', and a 'Font size:' dropdown set to '8'.

	R1	R2	R3	R4	Structure	Molecule Name	Synonyms	Sequence	Batch Name
1						ALT-0000449	c4mer-98825	F1NFQ1	1
2						ALT-0000448	c4mer-98824	F1NFR1	1
3						ALT-0000447	c4mer-98559	F1NYQ1	1
4						ALT-0000446	c4mer-98558	F1NYR1	1