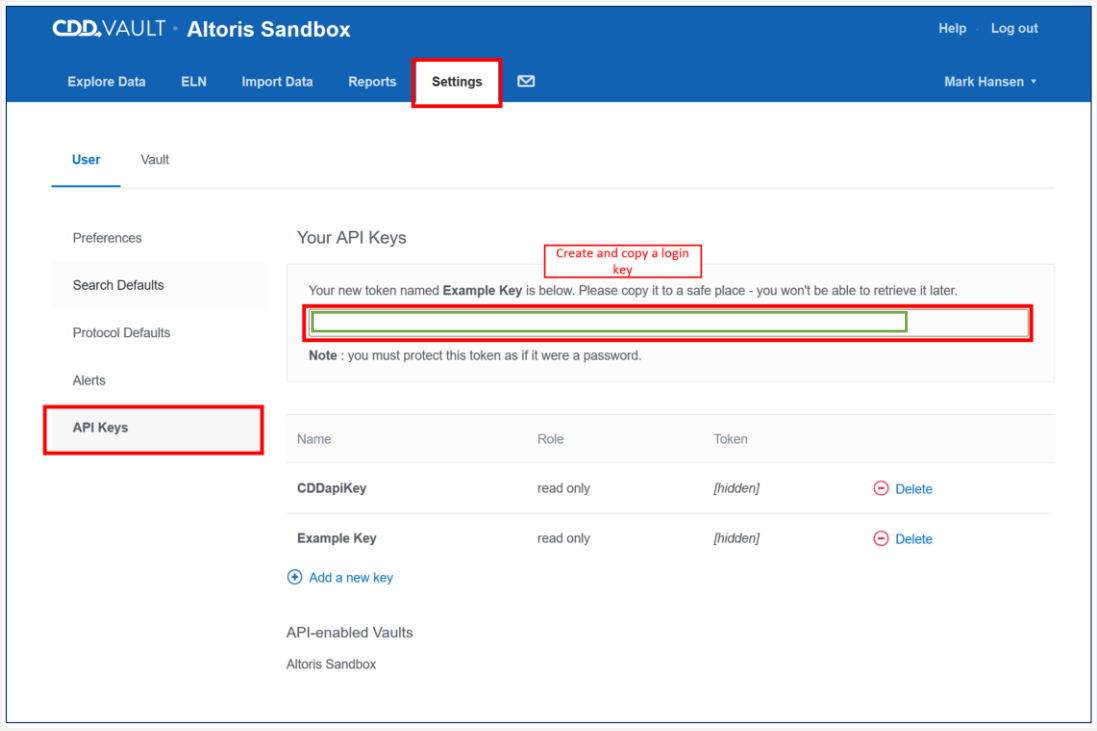
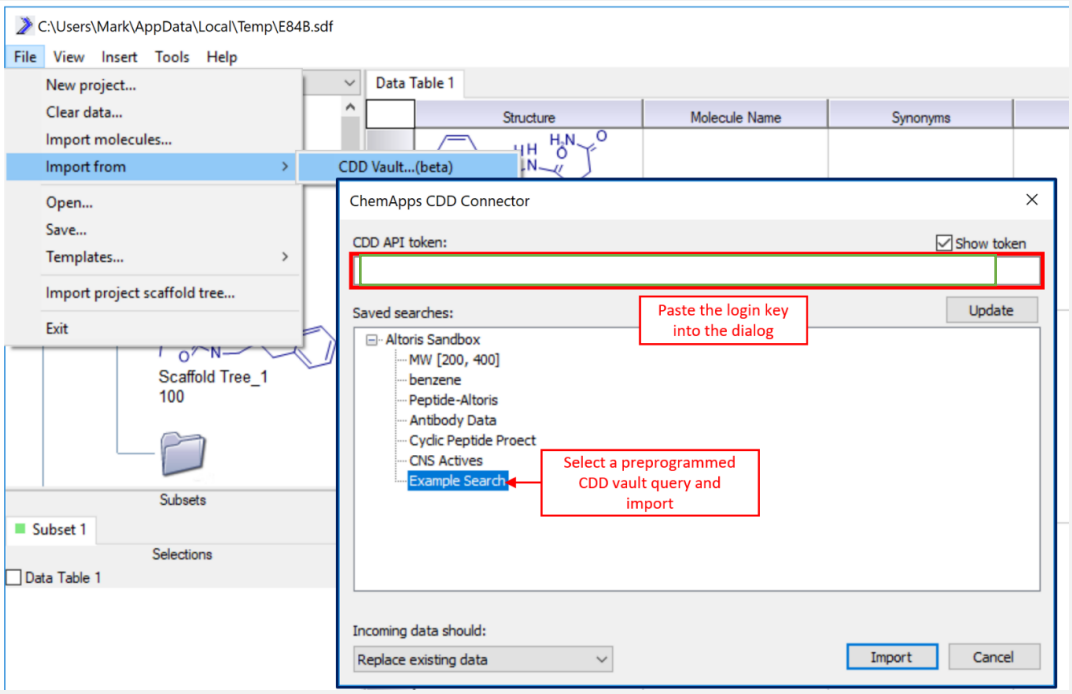
SARvision|SM and CDD Vault

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

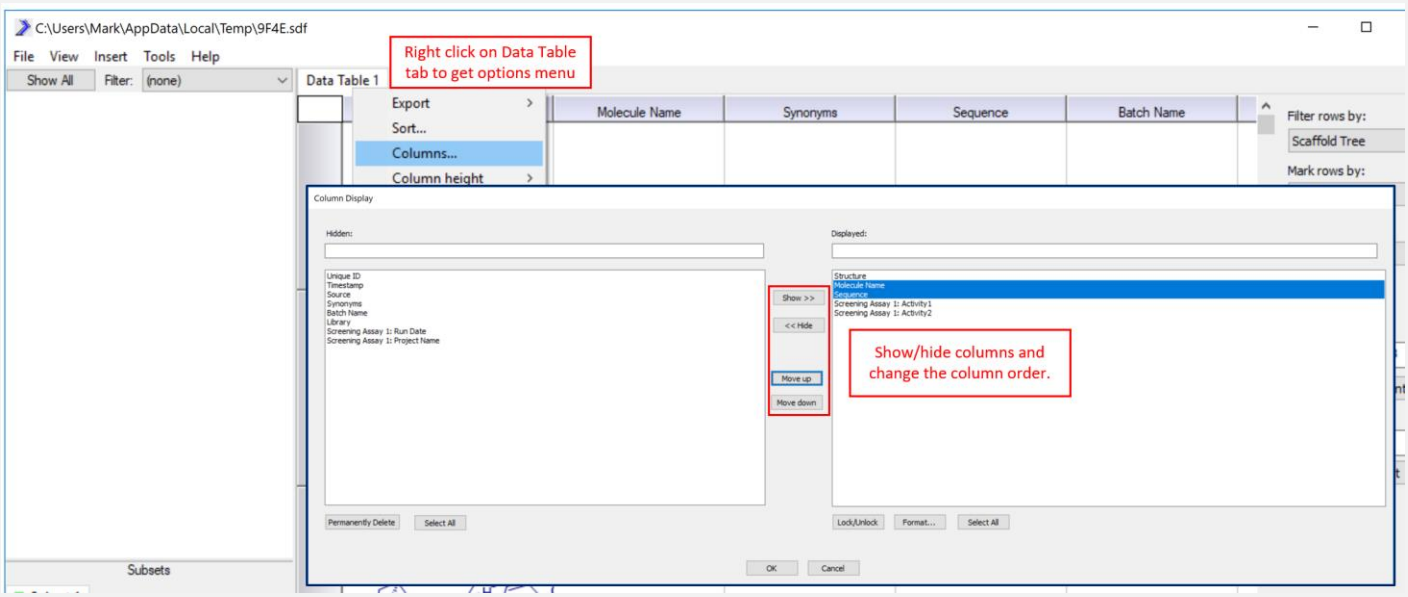
1. Log in to the CDD Vault and got to **Settings**. Under **API Keys**, *Add a new key* to use with SARvision. Copy this key so that it can be pasted into SARvision in the next step. This key contains all the information to allow SARivsion to have access to you CDD Vault database. Note that it can be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



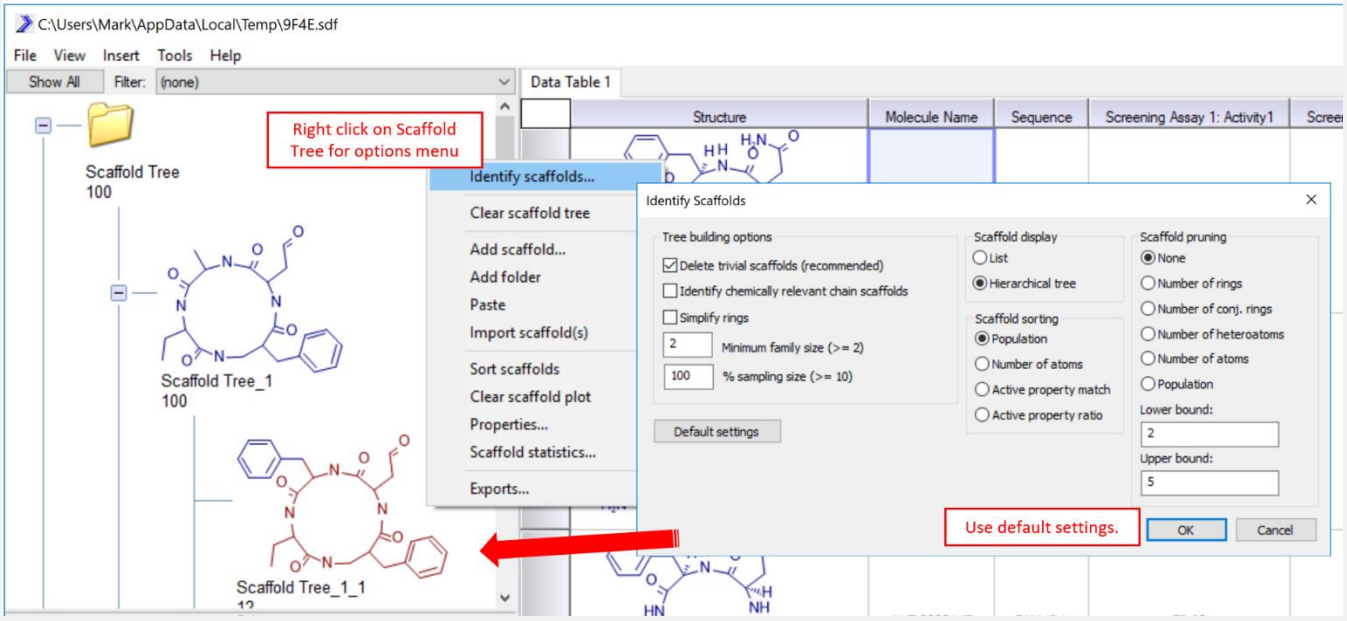
2. In SARvision|SM, under **File->Import from->CDD Vault…** paste the API token that you copied in step one into the correct box as shown. The Update button will reload the available saved queries in CDD Vault that you can access. If you do not have any, log onto CDD Vault and create some. In the ChemApps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



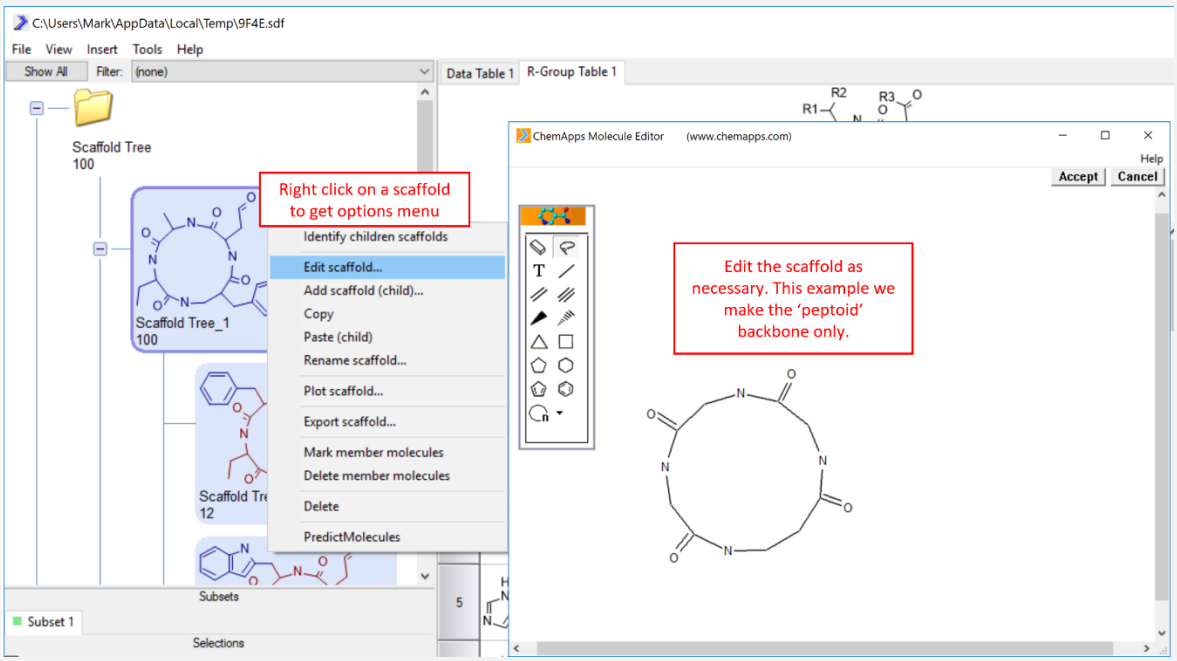
3. Once you have loaded some data, right click on the Data Table tab and use the **Columns…** control to clean up the table and show only the relevant columns.



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.



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.



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.