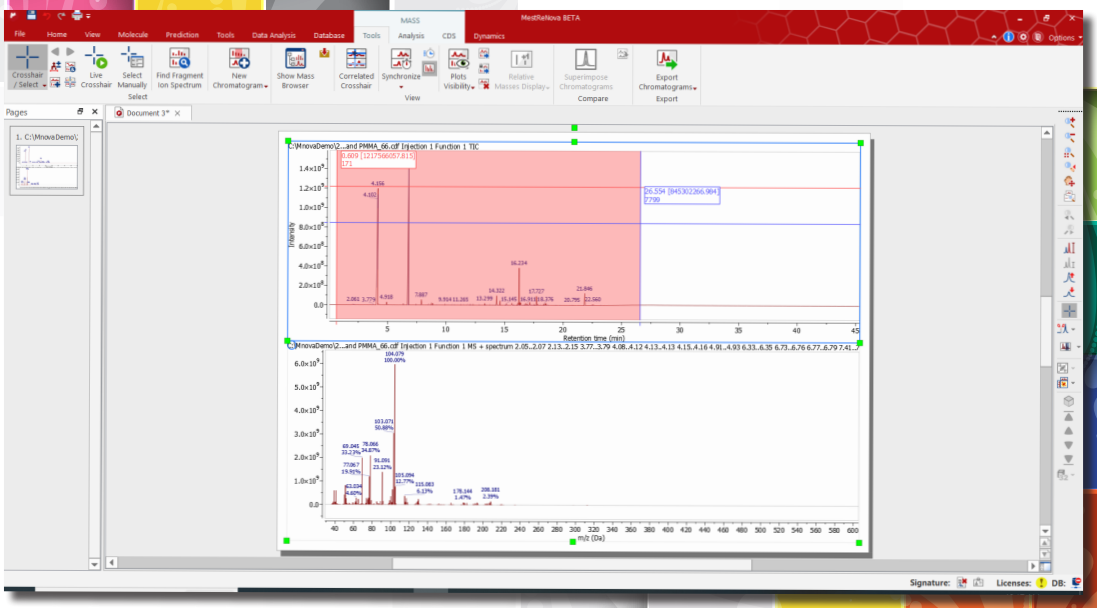
MSChrom and Database Manual



CDS Analytical
A LabTech Company

July 2024 Version

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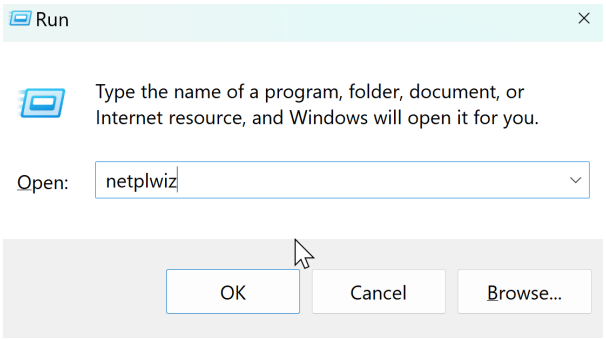
Introduction MSChrom CDSPlugin and Database Portal

Pyrograms are often complex and can be difficult to interpret. MSChrom with the CDS Plugin and MyData is a combination of chromatographic processing software including a database portal and search engine specifically designed for Py-GC-MS and EGA-MS data. It includes functions such as polymer identification, baseline correction, mixture deconvolution, and the ability to customize a database. Functionalities of different components are described in the table below :

Product	Part No.	Functionality
MSChrom with CDS Plugin	10A1-3027	Py-GC-MS data analysis and database search software. Includes a single nominated or workstation license for perpetual (lifetime) Mnova MSChrom, Database and MyData with customized functions, such as baseline correction and compound subtraction. Capable of accessing the NIST library search which needs to be purchased and installed on the same PC. Compatible with mainstream GC-MS file formats including Thermo, Agilent, Shimadzu and PerkinElmer. A microplastic library of 12 polymers and a NIST additive library of 260 compounds, as well as a customizable database build using MyData included.
EGA-MS database	10A1-3025	Evolved Gas Analysis(EGA) full MS data including Total Ion Current and full Mass Spectra for over 600 polymers. Compatible with MSChrom search and data processing software, which needs to be purchased separately.
Py-GC-MS database	10A1-3026	Pyrolysis(PY)GC-MSdata including Total Ion Chromatogram and Mass Spectrum instead of averaged mass spectrum for over 600 polymers as a polymer identification tool. The data is compatible with MSChrom search and data processing software, which needs to be purchased separately.
All-In One	10A1-3027	MSChrom plus CDSPlugin Py GC-MS Data Analysis Software EGA database of over 600 Polymers Py database of over Polymers

System Requirements

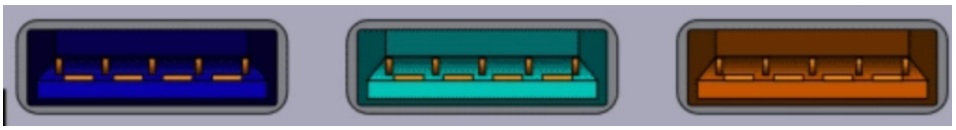
- **User has Administrator rights on the computer. To test if you have Administrator right, press the Windows key + R, then type netplwiz, then click OK. If the User Accounts window appears, you're logged in as an administrator. If you see a prompt to enter your credentials, please see IT to make you to be the administrator.**



- **Minimum Operation System: Windows 10**

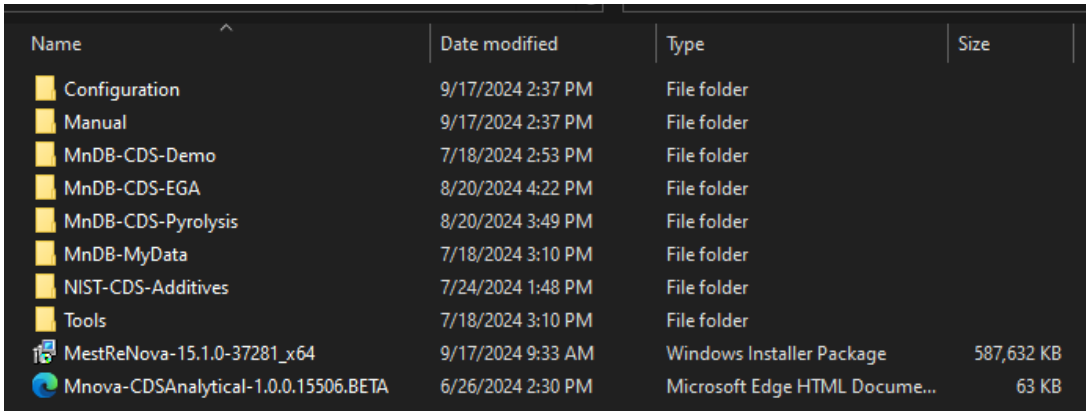
- **Minimum CPU: I5 9th Gen**

- **Dedicated (not through hub) high Speed USB 3.0/3.1/3.2 port required. Please look for a colored usb port in blue, green or red, or a black USB port with SS (superspeed) mark.**



External Drive Contents

Depending on your product purchase, you will have been given an external hard drive containing installers for MSChrom with CDSPlugin that includes the Microplastics Py-GC-MS, EGA and additive databases, full EGA-MS database (if purchased) and a full Pyrolysis-GC-MS database (if purchased).

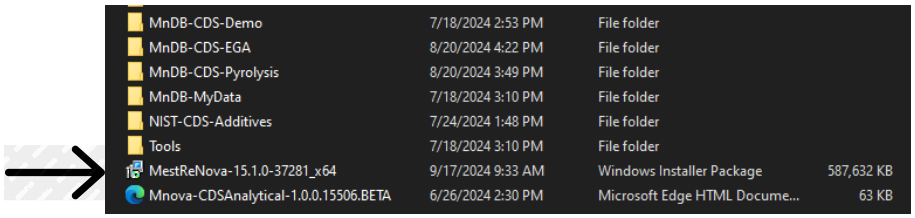


File/Folder	Description
Configuration	Integration and Database Configuration files
Manual	MSChrom Manual
MnDB-CDS-Demo	Microplastics Py-GC-MS and EGA databases.
MnDB-CDS-EGA	EGA database
Mn-DB-CDS-Pyrolysis	Pyrolysis database
MnDB-MyData	DIY database
NIST-CDS-Additives	NIST database of additives
Tools	Optional Items
MestReNova-15.1.0-37281_x64	Installer for MSChrom software
Mnova-CDSAnalytical-1.0.0.0.15506.BETA	CDSPlugin for MSChrom

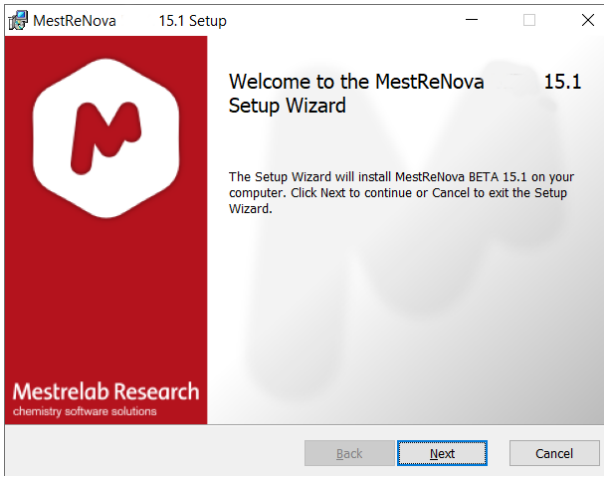
MSChrom Installation

Insert the hard drive into the high speed usb 3.0/3.1/ or 3.2 port. This port will now be the dedicated port for the database. The databases can not be accessed if the hard drive is switched to a different port.

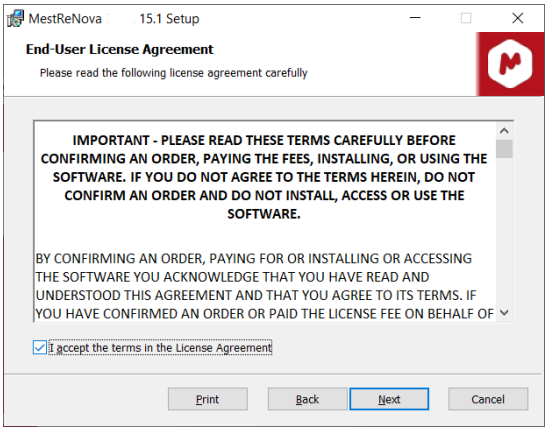
Double-Click the installer icon "MestReNova-15.1.0-37281_x64"



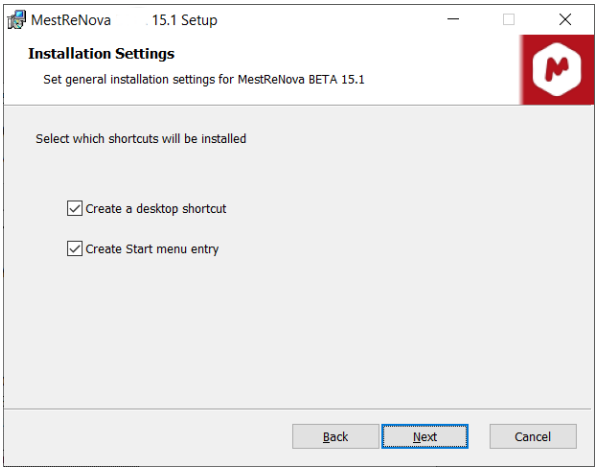
Click "Next" on the Setup Wizard Introduction Window.



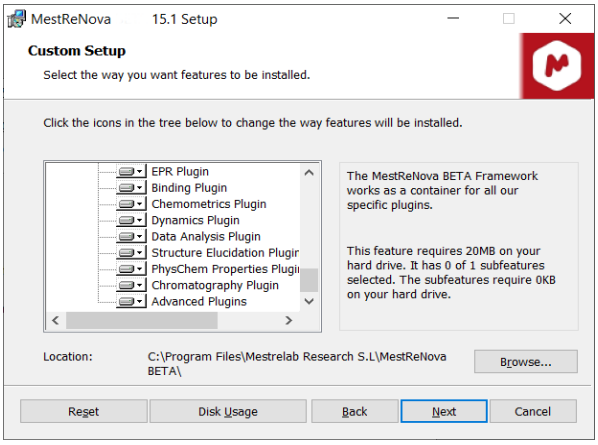
Accept the Agreement and choose "Next"



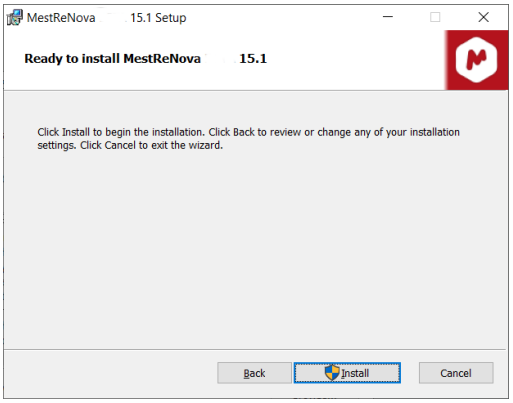
Click “Next” through the following windows.

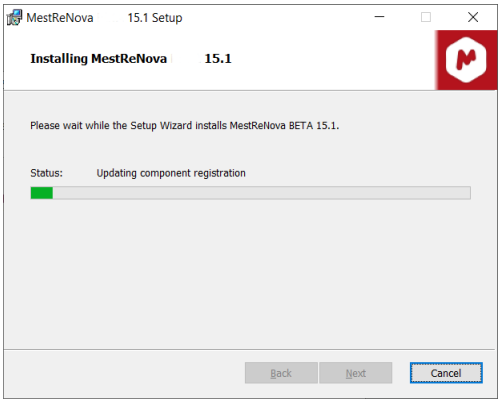


Click “Next” on the Custom Setup.

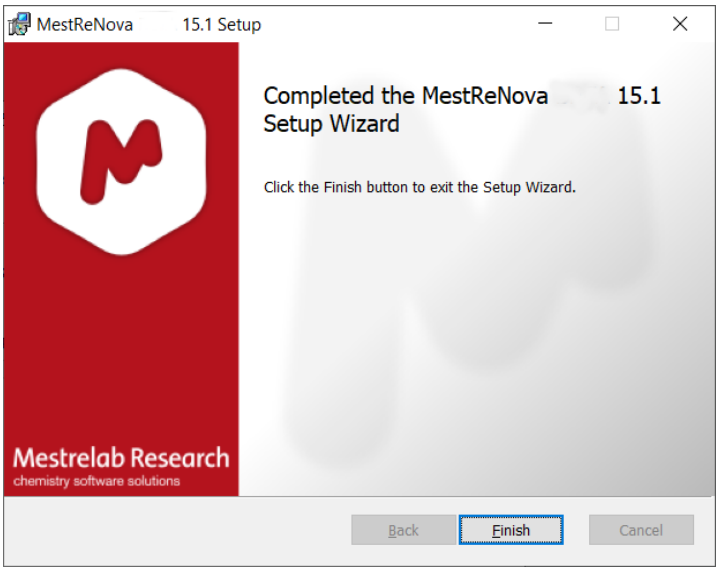


Choose Install on the next screen, and the software will install.

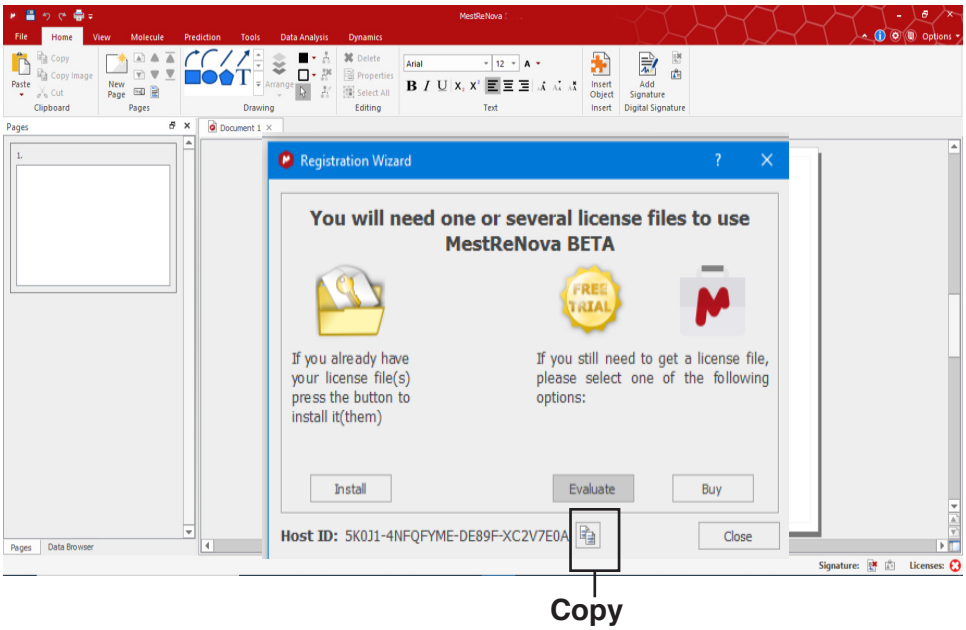




Click Finish, to finish the Installation.

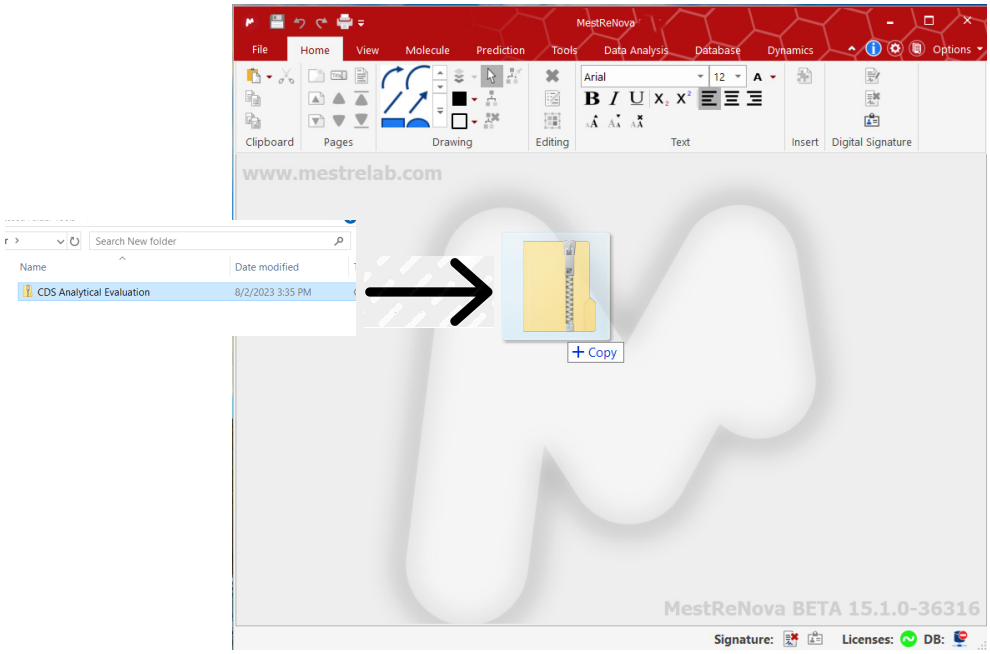


License Files MSChrom CDS Plugin & Databases



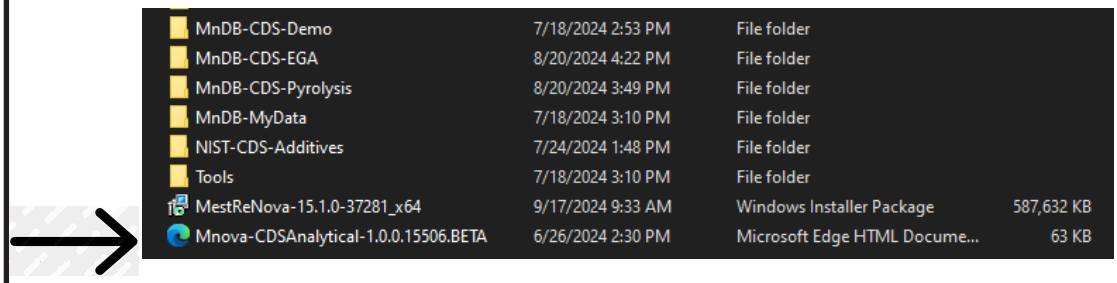
Double click on the Mnova ICON to open the software. When it is opened for the first time, you will be prompted for a license file. Copy the HOST ID, close the window, and paste the ID in an email to webmaster@cdsanalytical.com with the purchase order number to request appropriate licenses. Licenses are needed for MSChrom, the EGA and Pyrolysis databases, and the CDS Plugin.

Once a licenses for MSChrom and the CDS Plugin are aquired, drag the folder into MSChrom.

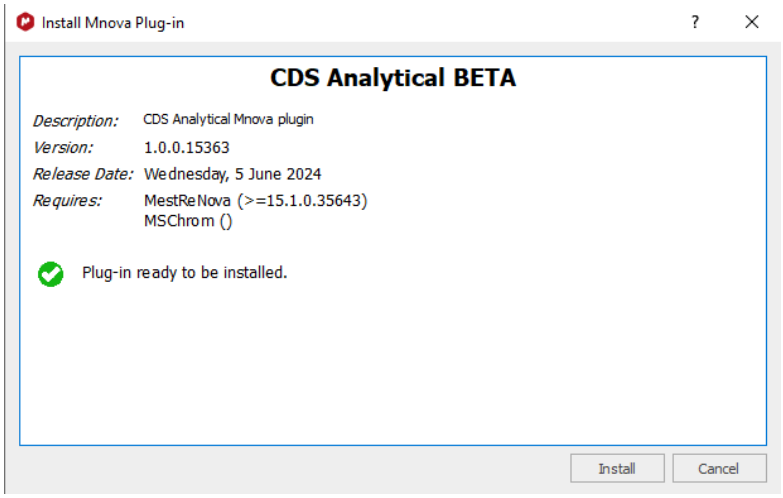


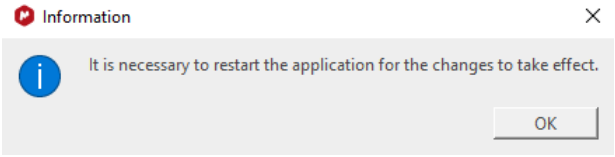
CDSPlugin Activation

Activate the CDS Plugin by dragging the Mnova-CDSAnalytical-1.0015506. BETA file from the external drive into MSChrom.

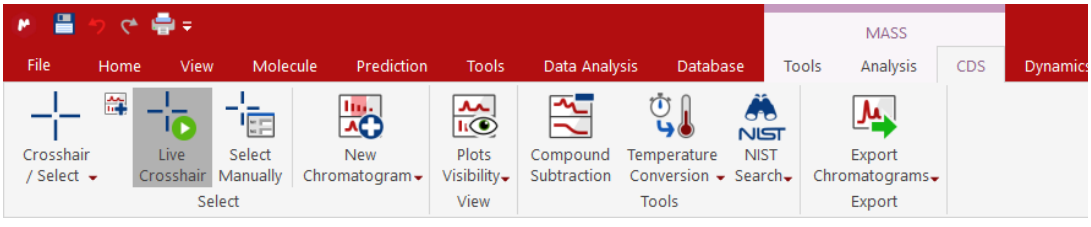


This below dialog window will appear. Select "Install"





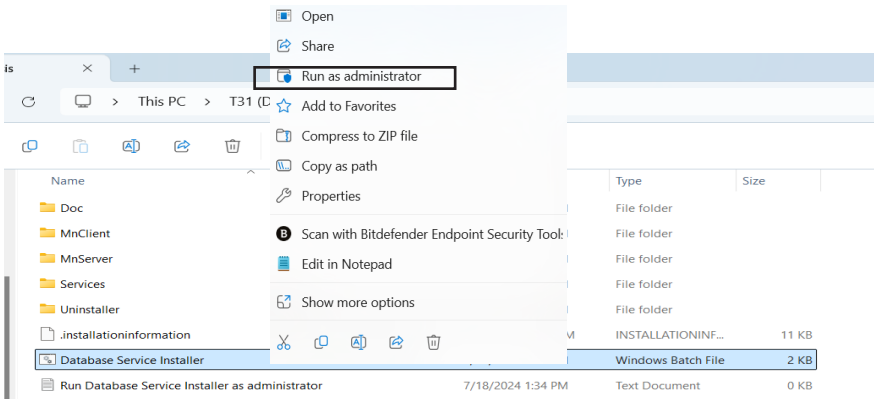
Click "OK", close MSChrom and re-open it to activate the CDS Plugin. Drag a chromatogram datafile into MSChrom, the CDS Ribbon will be shown as:



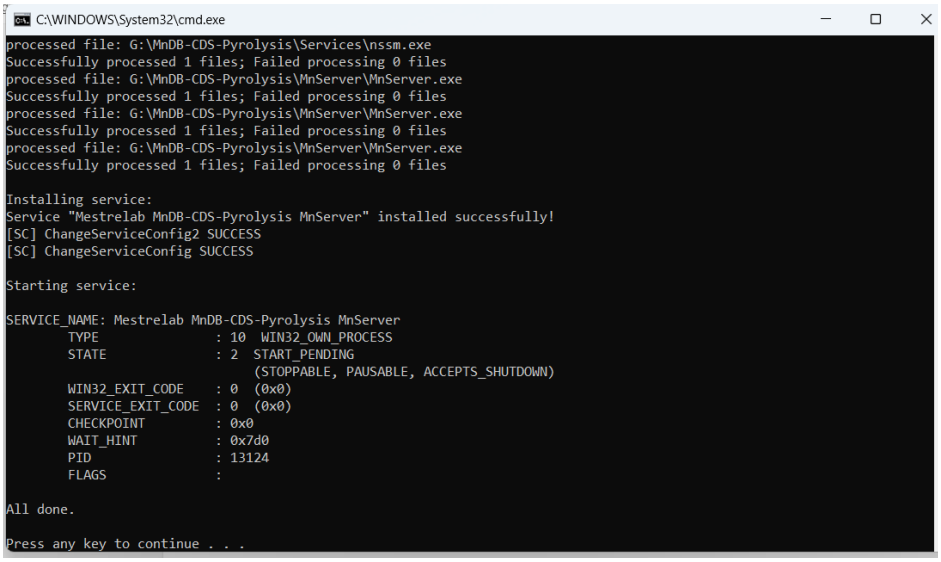
Once MSChrom & CDSPlugin and Database license files (.lic) are recieved, drag them into MSChrom to activate.

Included Database Installation/ Activation Microplastic Py & EGA

The Microplastic Py & EGA Databases will not require a license. Right Click the "Database Service Installer" icon in the MnDB-CDS-Demo folder and select "Run as Administrator".



A black screen will open, documenting the Services installation.



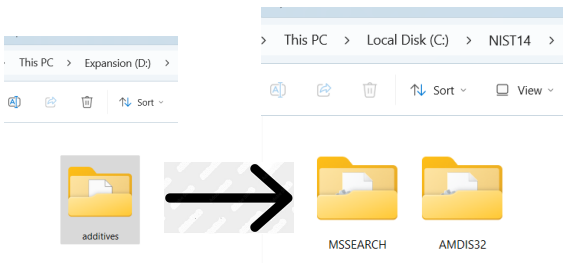
Once it has finished, close the window. Now the database service is installed for the Microplastic EGA & Pyrolysis Databases.

My-Data

The My-Data Database does not require a license. Right Click the "Database Service Installer" icon in the MnDB-CDS-Demo folder and select "Run as Administrator", as described above for the Microplastic Py & EGA Databases.

NIST Additive

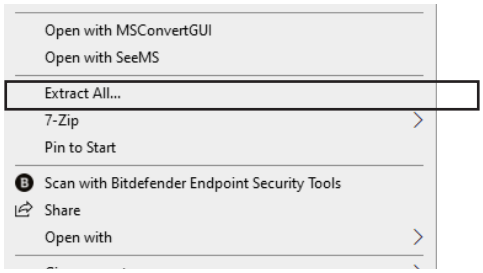
The NIST library contains EI MS spectra for over hundreds of thousands small molecules. When searching additives in the pyrogram, the NIST library is an excellent tool to identify individual peaks of interest even when these peaks are not contributed by additives. The CDS additive library is designed in such a way to blend into existing NIST libraries. To install, copy the additives folder from the external drive, and place it in the MSSearch Folder of the NIST folder on the local drive.

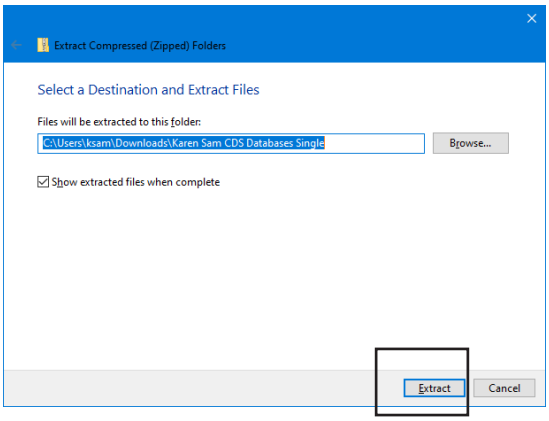


Optional Database Activation Pyrolysis & EGA

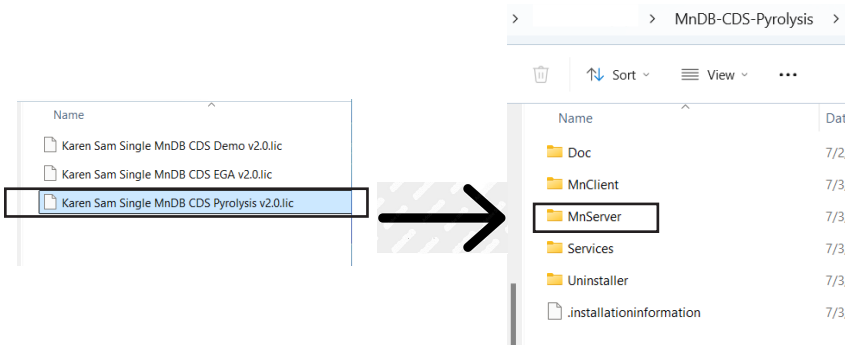
The CDS Pyrolysis and EGA databases are fully installed on the supplied external hard drive, and need to be activated. The USB port needs to be dedicated to this external hard drive. Databases cannot be accessed if the hard drive is switched to a different port.

The first step of database activation is to activate the licenses. Once the license files are obtained from in a zip folder from CDS Analytical, right-click the folder and choose "Extract All", then press "Extract."

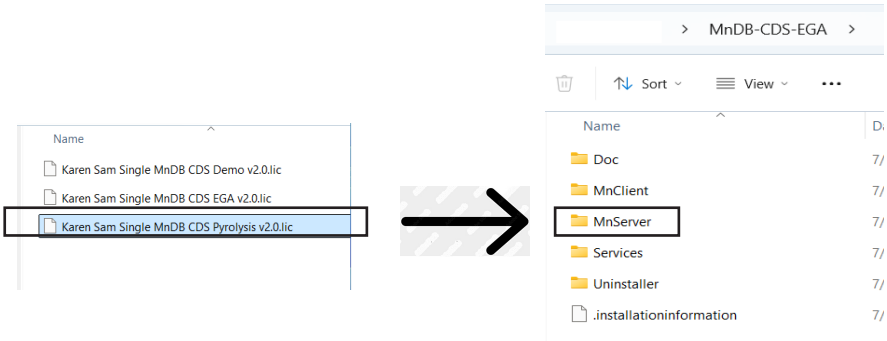




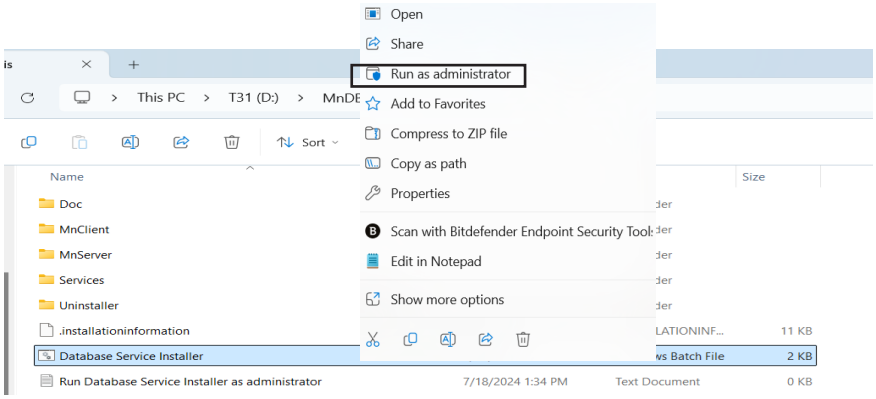
Copy the Pyrolysis database license (.lic) into the MnServer folder of the MnDB-CDS-Pyrolysis folder of the external drive.



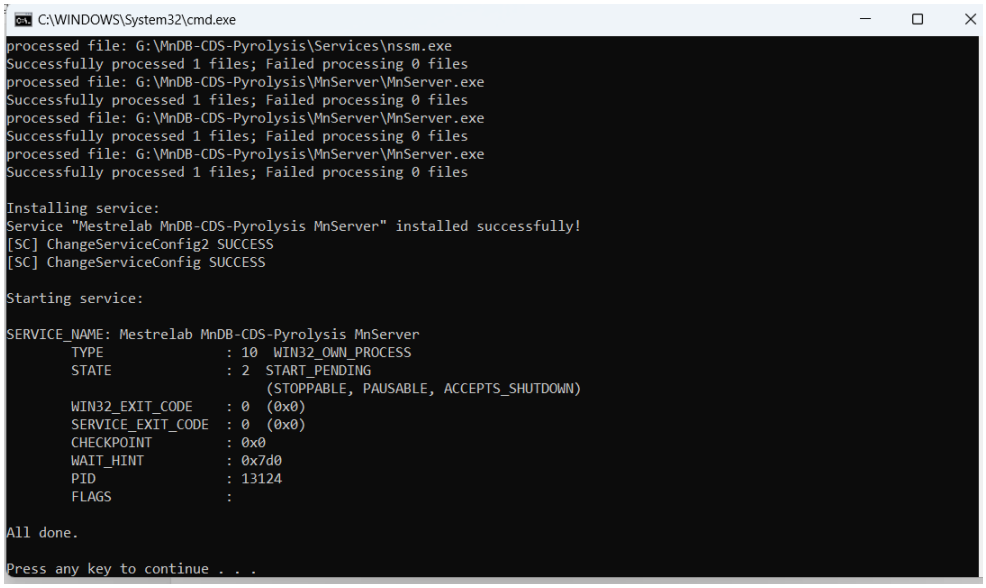
Copy the EGA database license (.lic) into the MnServer folder of the MnDB-CDS-EGA folder of the external drive.



Second, right click the “Database Service Installer” icon in the MnDB-CDS-Pyrolysis folder and select “Run as Administrator”.



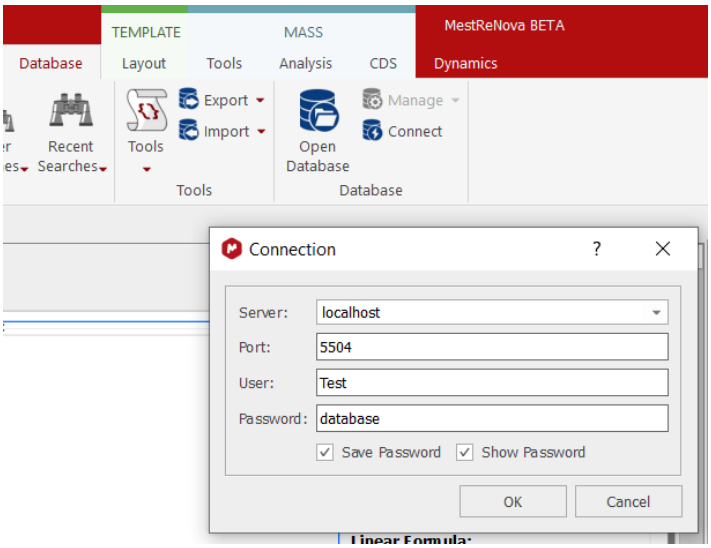
A black screen will open, documenting the Services installation.



Once it has finished, close the window. Now the database service is installed for the Py database. Repeat the above process in the MnDB-CDS-EGA folder to activate the EGA database.

Listening Ports

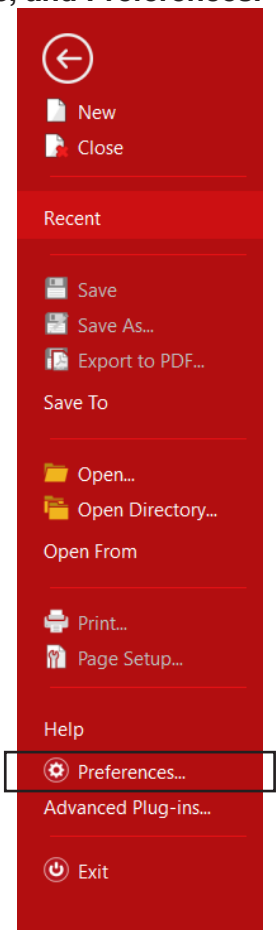
Each Database is configured to different Listening Ports. When using MSChrom, you will need to connect to the corresponding listening port in the database tab to access the proper database. The table below lists the listening ports and login credentials. This will be further covered in the "4 Steps to Searching the Database" Section.



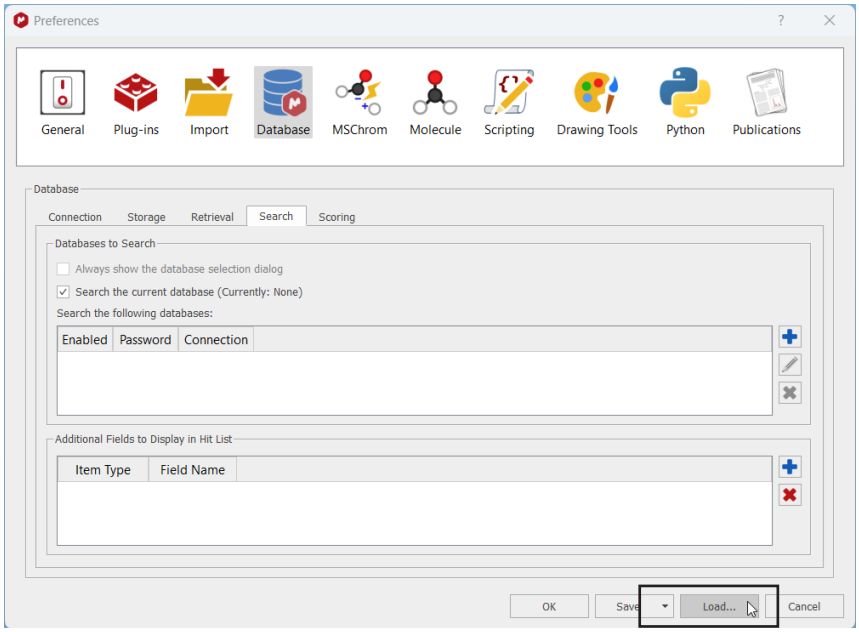
Database	Listening Port	UserName	Password
CDS Demo (Microplastic)	5533	Test	database
Pyrolysis	5532	Test	database
EGA	5531	Test	database

Database Search Configuration

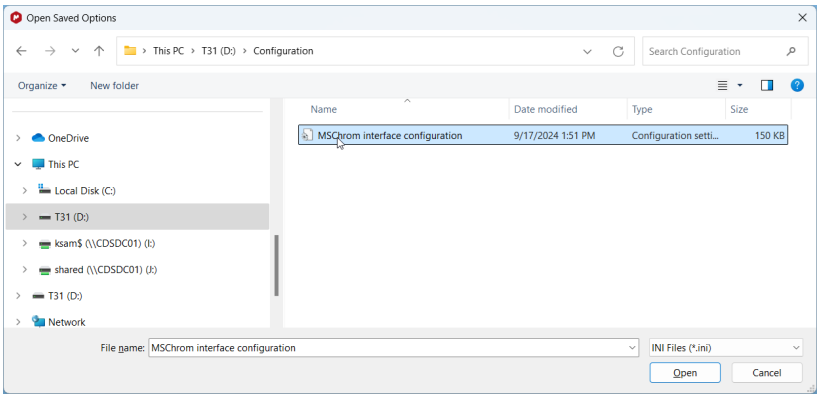
The database settings need to be configured to display the Polymer Name in the Search Results. This can be done by loading a file in Preferences. In MSChrom. Choose File, and Preferences.



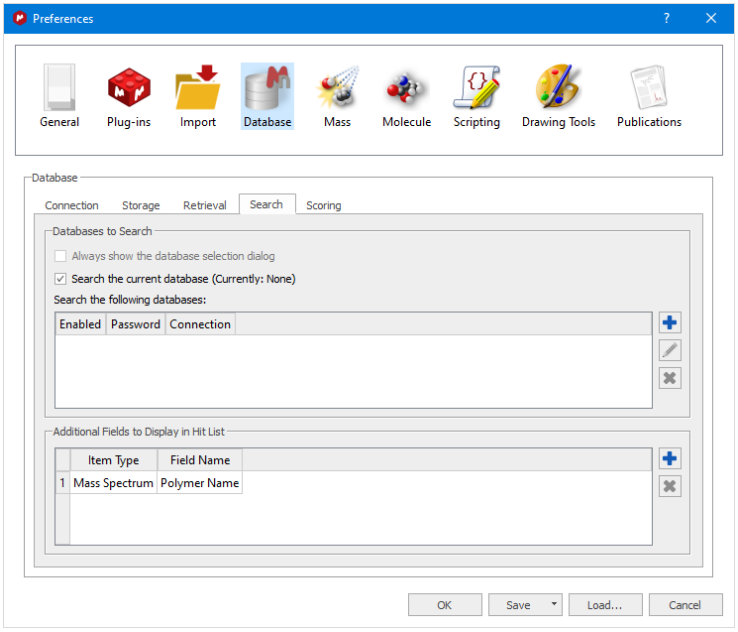
Pick the Database icon, and the Search Tab. Click on "Load." Navigate to the "MSChrom interface configuration under the Configuration Folder on the External Hard Drive.



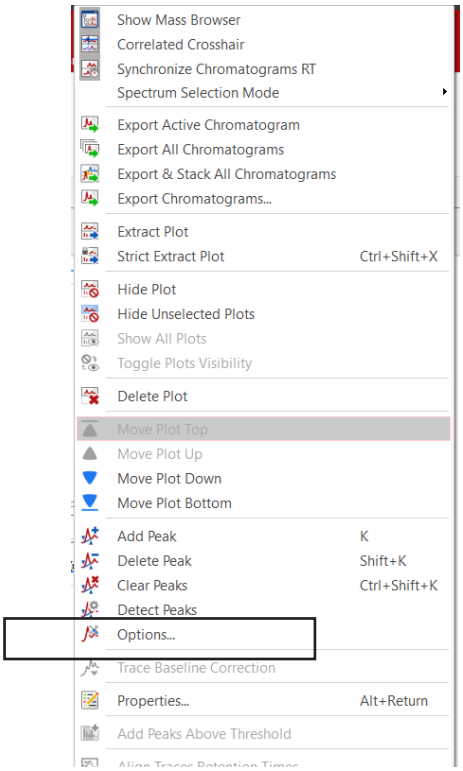
Navigate to the “MSChrom interface configuration” under the Configuration Folder on the External Hard Drive.

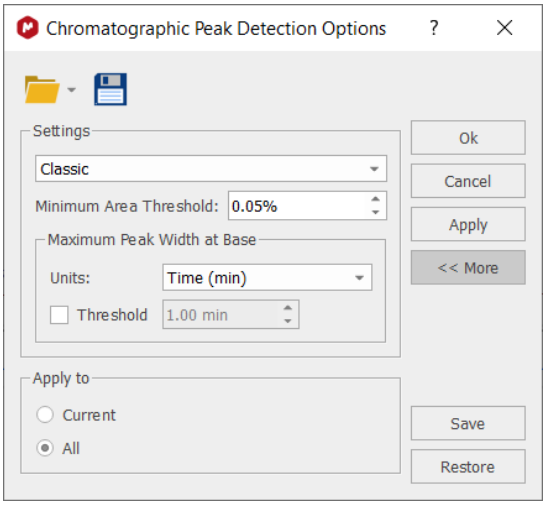


Now the Polymer Name Field will appear in Polymer Search Hit Lists.



Drag a data file into MSChrom to modify the Integration settings. Integration Settings such as the integration threshold needs to be optimized for PY-GC-MS data by right-clicking over the chromatogram, and choosing “Options”





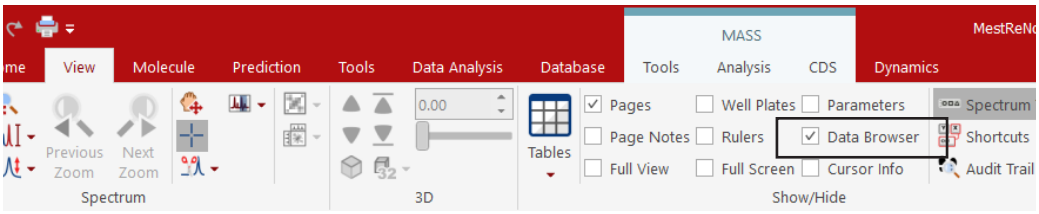
There are two Integration setting types, Classic and Enhanced.

Minimum Area Threshold is defined as the minimum percentage of the total area of all the identified peaks in the chromatogram. The Py-GC-MS database was acquired using a 0.05% Threshold with a Classic Integration.

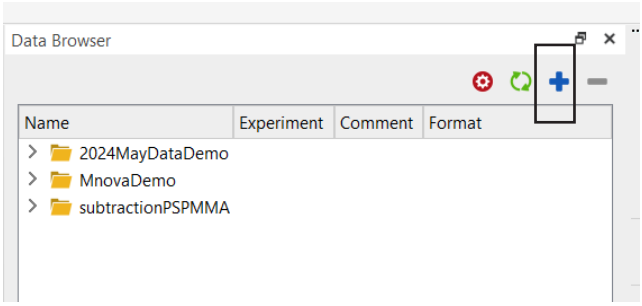
Hit “Apply” to apply any changes, and “Save” to save those changes.

MSChrom Operation

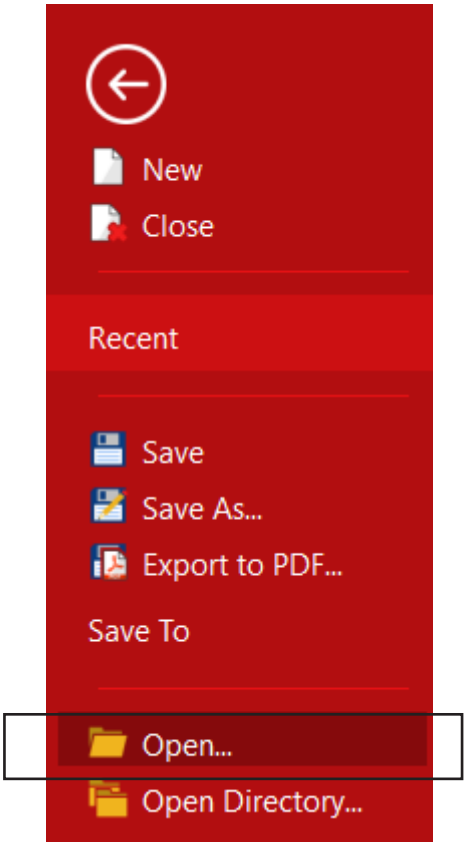
Py-GC-MS data can be brought into MSChrom by several ways. One way is to drag a file into the MSChrom browser from Windows File Explorer. A second way is to use the Data Browser. The Data browser can be displayed by checking the box next to “Data Browser” in the “View” Ribbon.



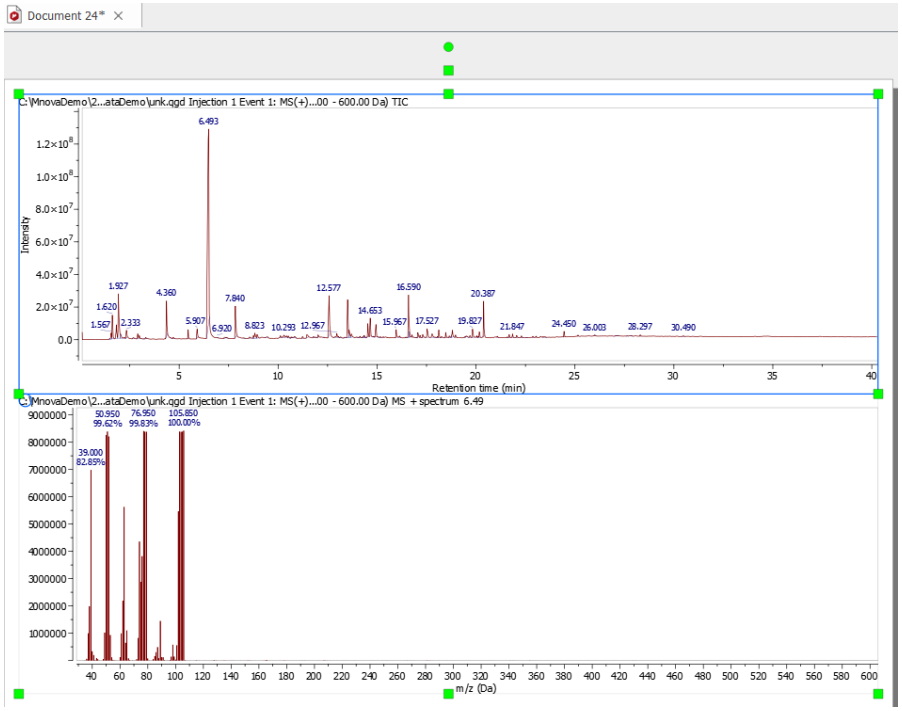
File locations can be added to the browser by choosing the blue plus symbol. GC-MS files can be dragged into a new or open document from this Data browser



A third way is to choose File from the top menu, then Open.



When files are opened, chromatograms will be loaded with peaks integrated. As a default, the mass spectrum of the highest peak will be displayed under the chromatogram.



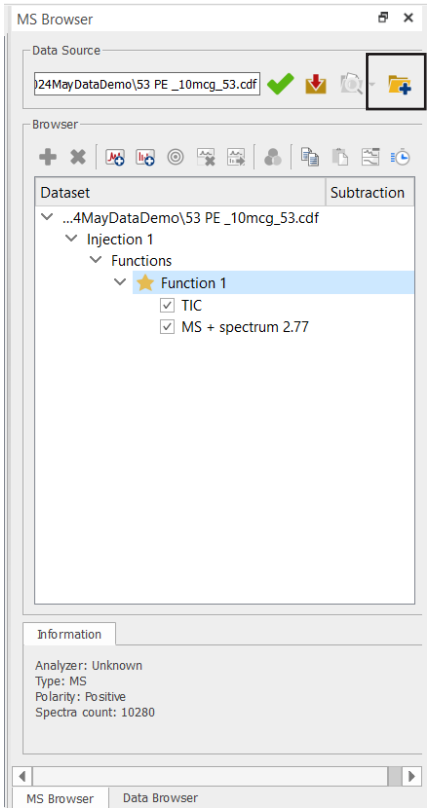
All Py-GC-MS data entries were pyrolyzed at 700°C for 30 seconds. The GC column was a 30 meter 5% phenyl with a 0.25mm I.D. and a 0.25*μ*m film thickness.

4 Steps to Search the Pyrolysis Database

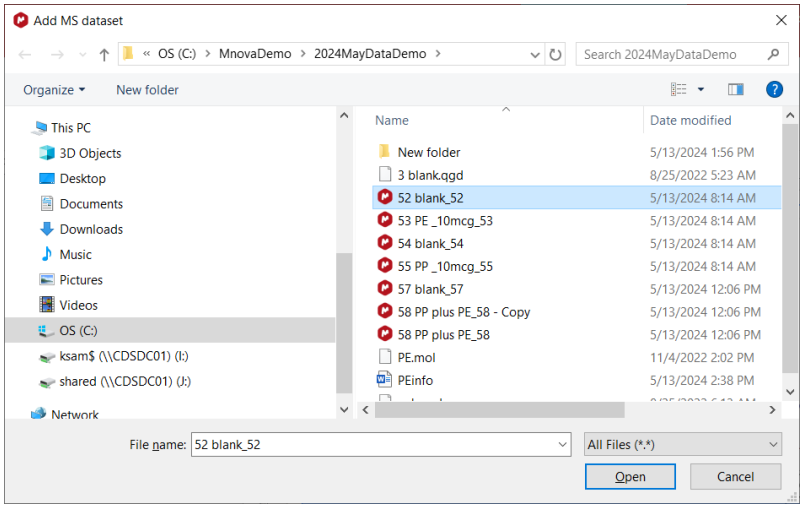
Step 1: Baseline Correction

Once data is loaded, it can be baseline corrected by deducting a blank TIC. this minimizes common background interference such as column bleed.

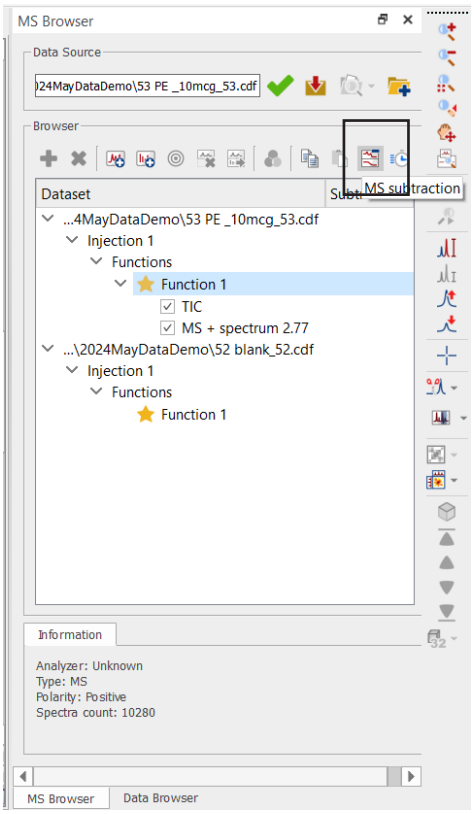
a. Click on the "Mass Browser" Tab and select the folder plus icon to add a second dataset to the browser.



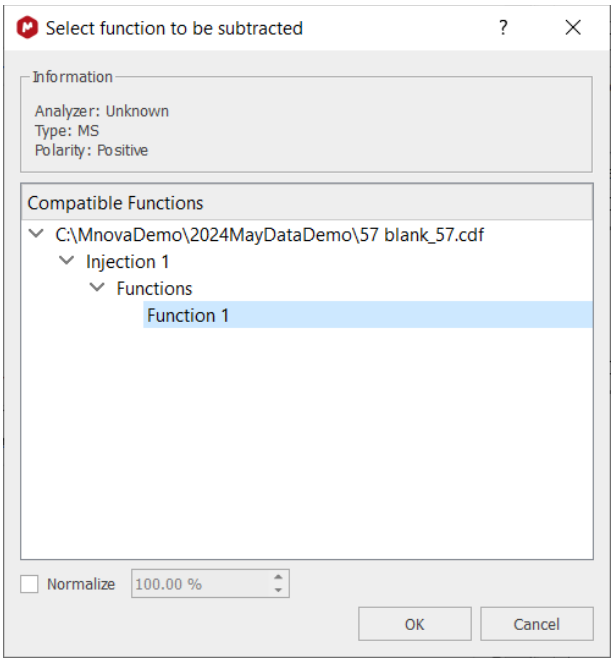
b. In the window that opens, select the blank data.



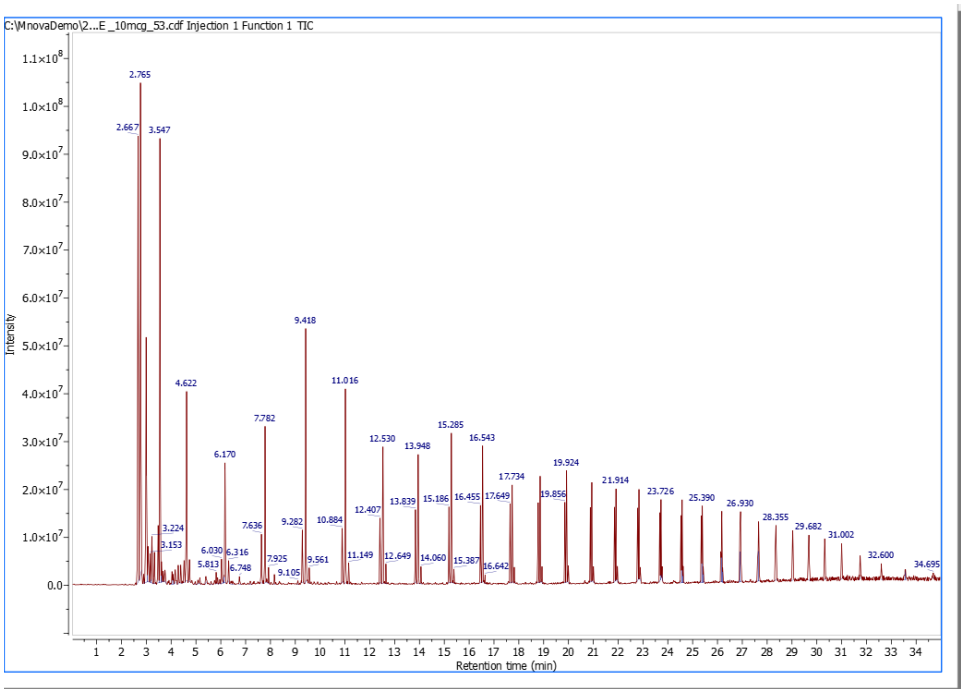
c. Once the blank data is loaded, highlight Function 1 of the sample data, and select the MS subtraction icon.



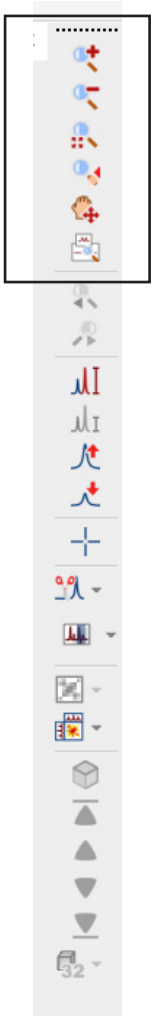
d. When the window "Select function to be subtracted" window opens, select Function 1 of the blank data, make sure the Normalize box is not checked, and click "OK".



Baseline corrected data will be calculated:

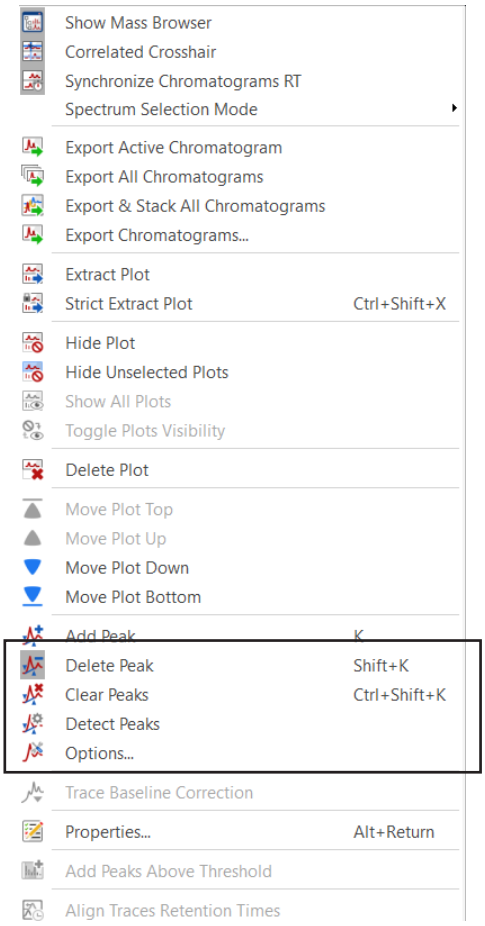


Zooming in and Out can be done by accessing the Quick Buttons on the right-hand side of MSChrom.



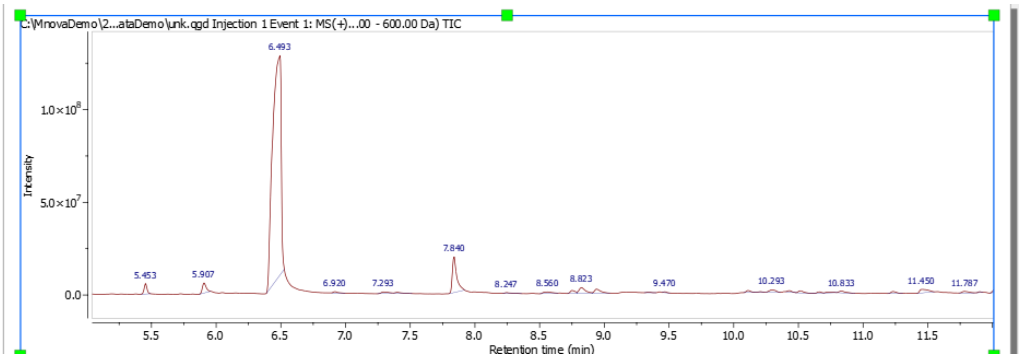
If there are is unwanted contamination or the need for a manual integration, the pyrogram can be adapted before co-adding the mass spectra for a database search:

Peak integrations can be removed, added, or re-integrated by right clicking on the chromatogram and one of the Peak Integration Icons, then dragging the cursor over the area that needs the change.

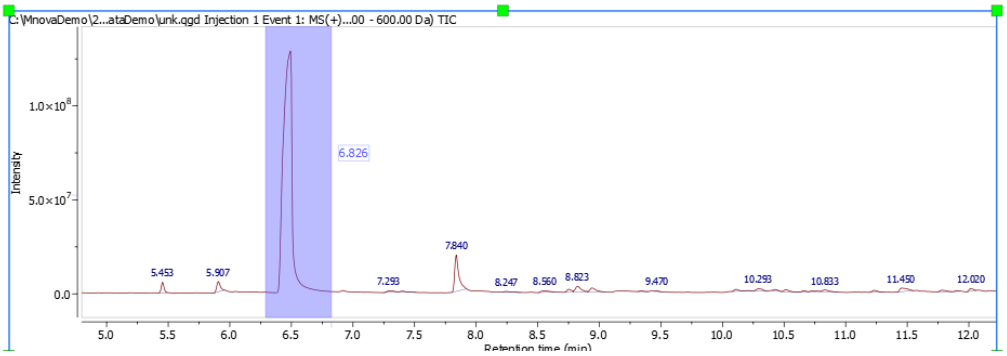


For example, to remove an integration, select “Delete Peak”, Then right-click and drag over the desired area. Once the peak integration is deleted, the retention time label and the integration line will disappear:

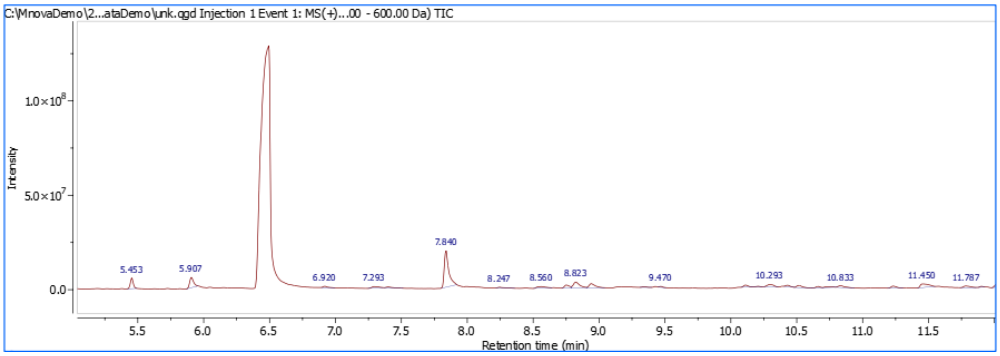
Before Deleting a Peak Integration:



Deleting a Peak Integration :

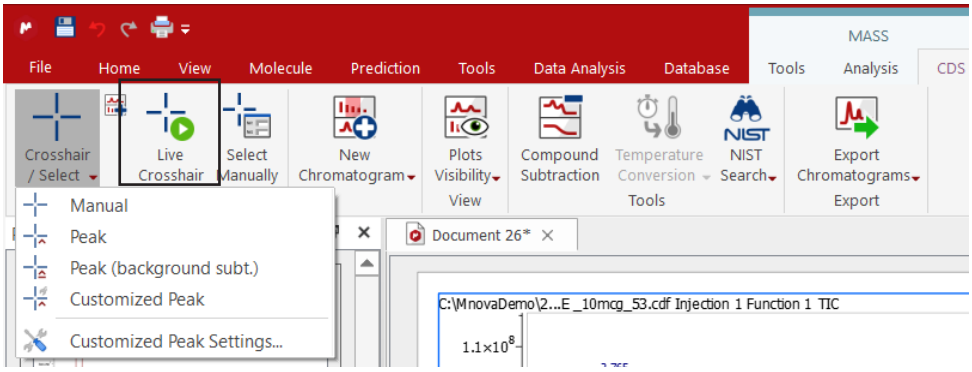


After Deleting Peak Integration:

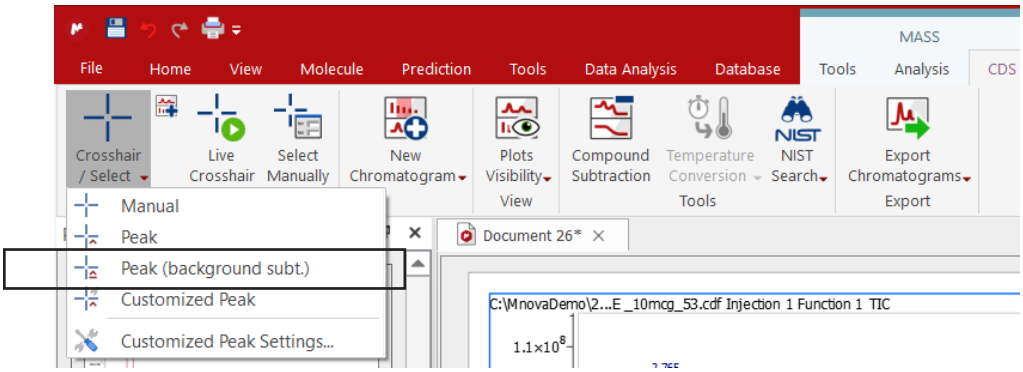


Step 2: Co-add Mass Spectra for Database Search

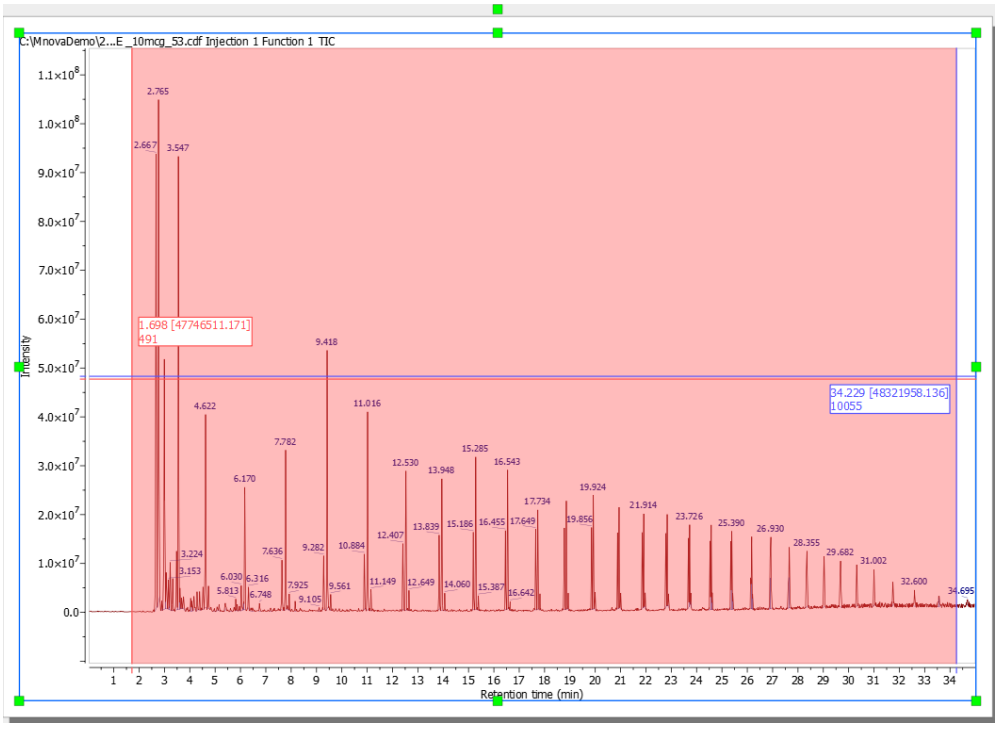
The Live Crosshair Tool shows a "live" mass spectrum changes as you drag your cursor along the chromatogram If you wish to de-select it, click on the Live Crosshair Icon. When an icon is not shaded grey, it means it is de-selected



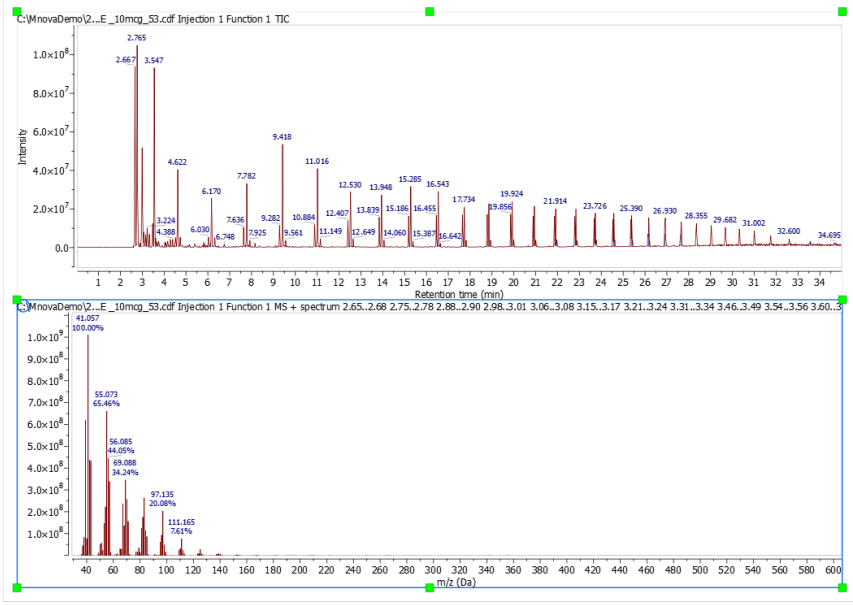
To co-add the Spectra, choose Peak(background subt) from the Crosshair Select Tool, under the CDS Ribbon. The Peak (background subt.) tool allows a user to select mass spectra of peaks to display, in which the tails of each peak are not included in the mass spectrum, to provide cleaner data.



After selecting this option, left-click and hold on the left side of the chromatogram, and then drag the mouse chromatogram to display the co-added mass spectrum under the chromatogram.

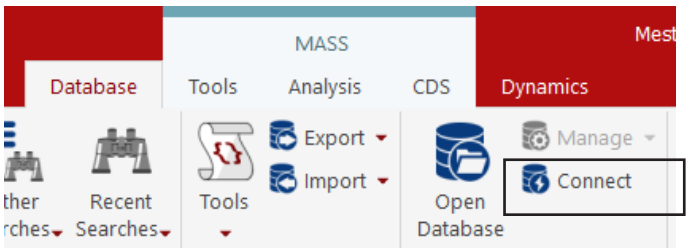


The co-added spectrum will appear below the chromatogram.



Step 3: Search Database

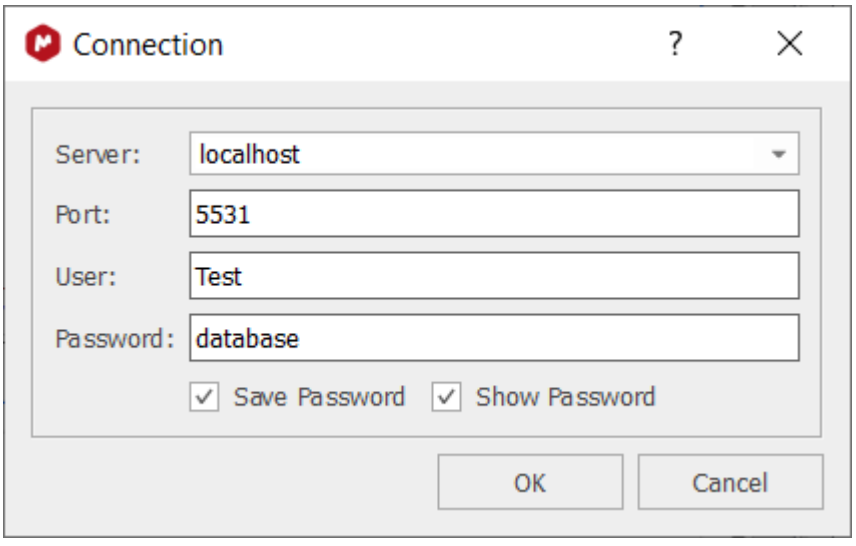
To first connect to the database, choose "Connect" under the database ribbon.



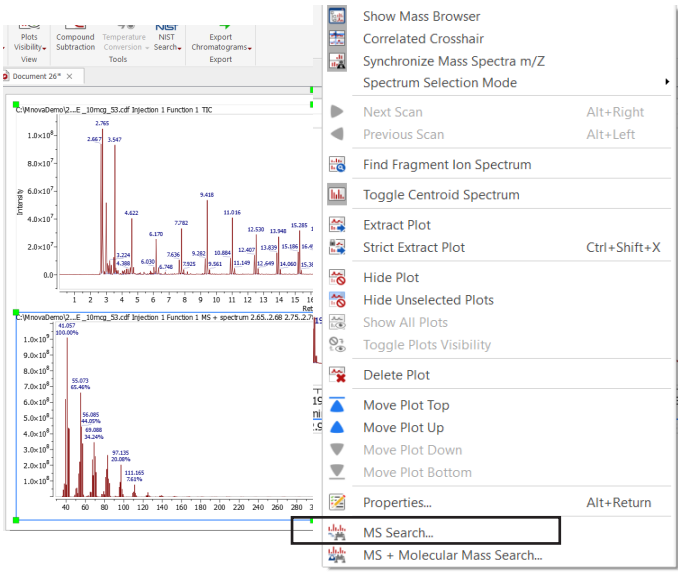
Each database uses a different Listening Port. Databases with their corresponding listening ports, usernames, and passwords are in the table below.

Database	Listening Port	UserName	Password
CDS Demo (Microplastic)	5533	Test	database
Pyrolysis	5532	Test	database
EGA	5531	Test	database

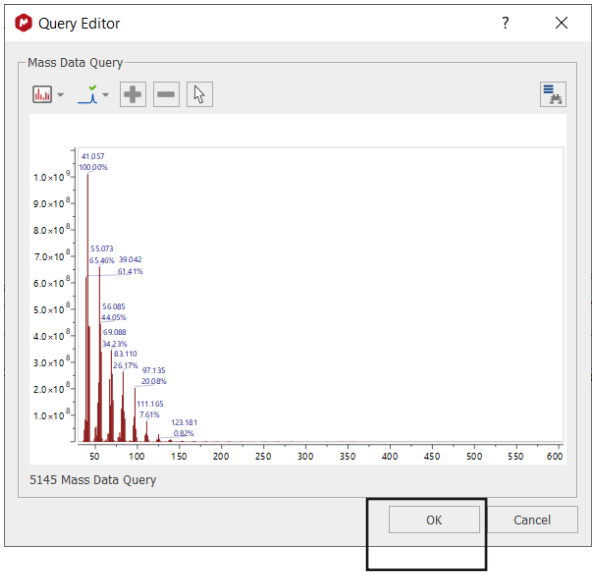
To search the Pyrolysis database, choose port 5532, enter the UserName and Password.



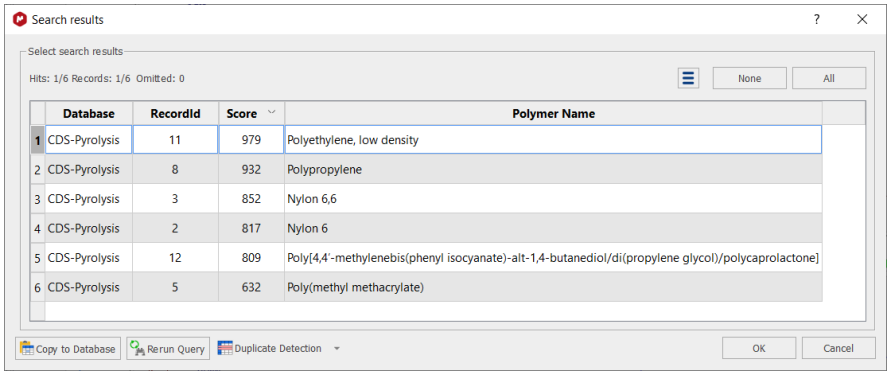
To Search the Pyrolysis Database, move the cursor over the co-added mass spectrum, right-click and choose “MS Search”



The Query Editor will open. Select “OK”.



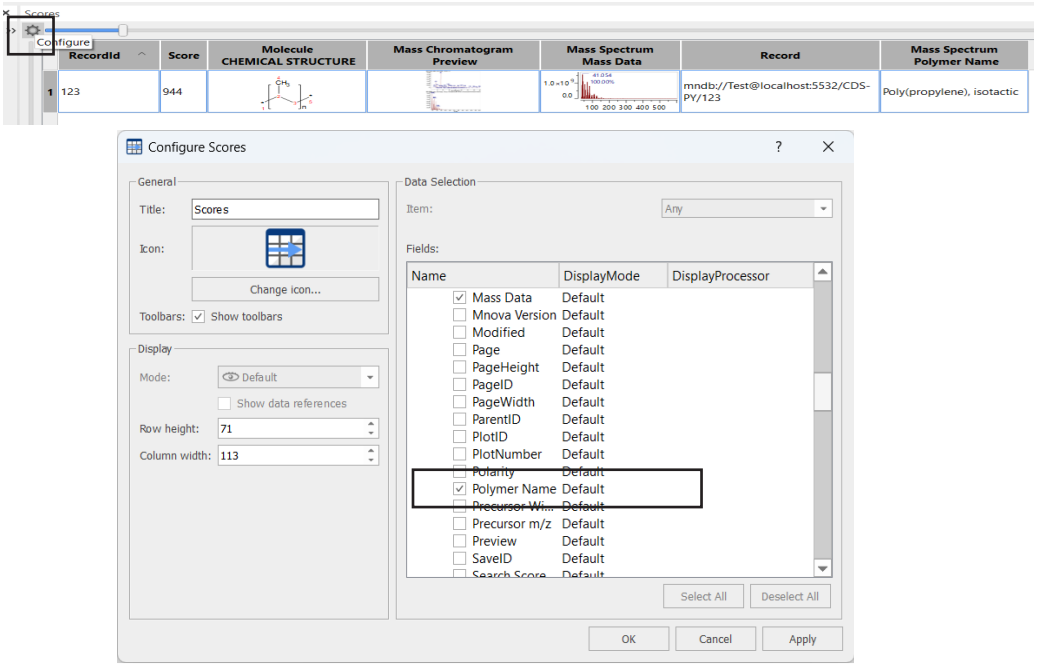
The search list will appear.



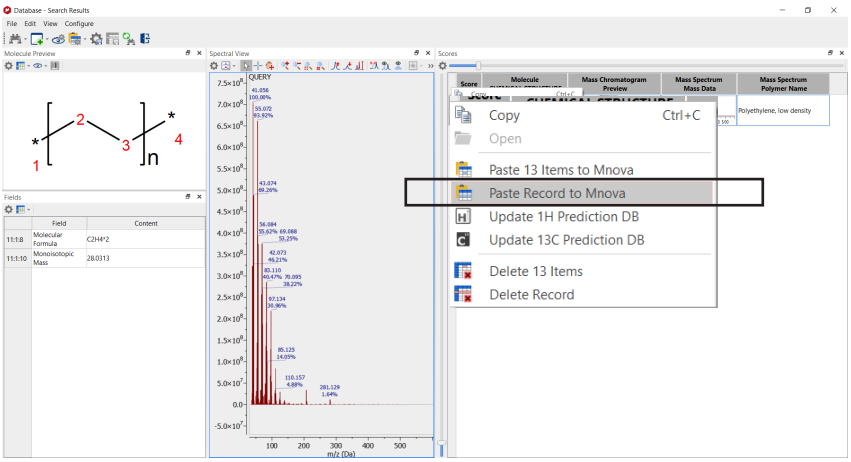
Click on any entry and select “OK” to open the database browser and view the entry in more detail.

Step 4: Compare Chromatograms

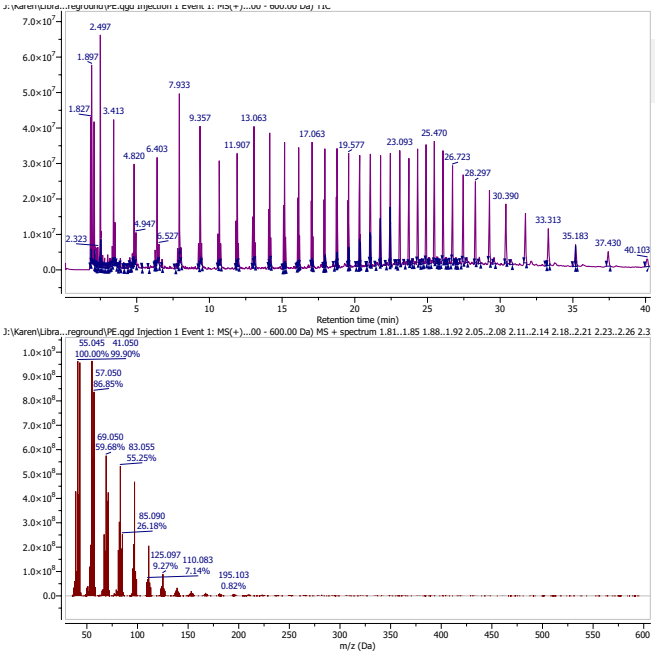
The first time the database browser opens, the Polymer Name field may not be shown in the scores section. You can add this field by selecting the Configure icon at the top left, then checking the Polymer Name Box after expanding the Mass Spectrum Category. Any field may be added or removed from this gear icon.



Select any desired entry. Multiple entries may be selected by holding down the “shift” key and selecting them in the search list. Select“OK’ to look at the matches in the database browser. To bring an entry to the MSChrom browser, right click on the entry in the Scores section, then select “Paste Record to Mnova”



Minimize the or close the DBbrowser window. Additional pages will appear in MSChrom document containing the database entries. Entries will include an integrated chromatogram, a co-added mass spectrum of all the peaks, any synonyms, CAS #, Polymer Names, Linear Formulas, Descriptions, and molecular structure.



Polymer Name:

Polyethylene, low density

CAS#: 9002-88-4

Linear Formula:

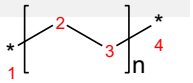
H(CH2CH2)nH

Synonyms:

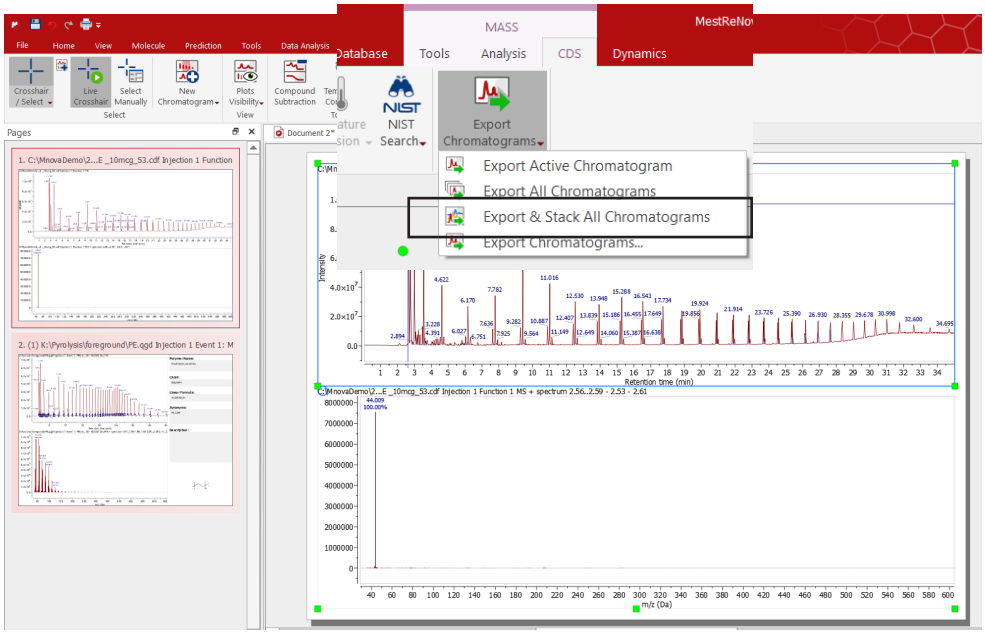
PE, LDPE

Description:

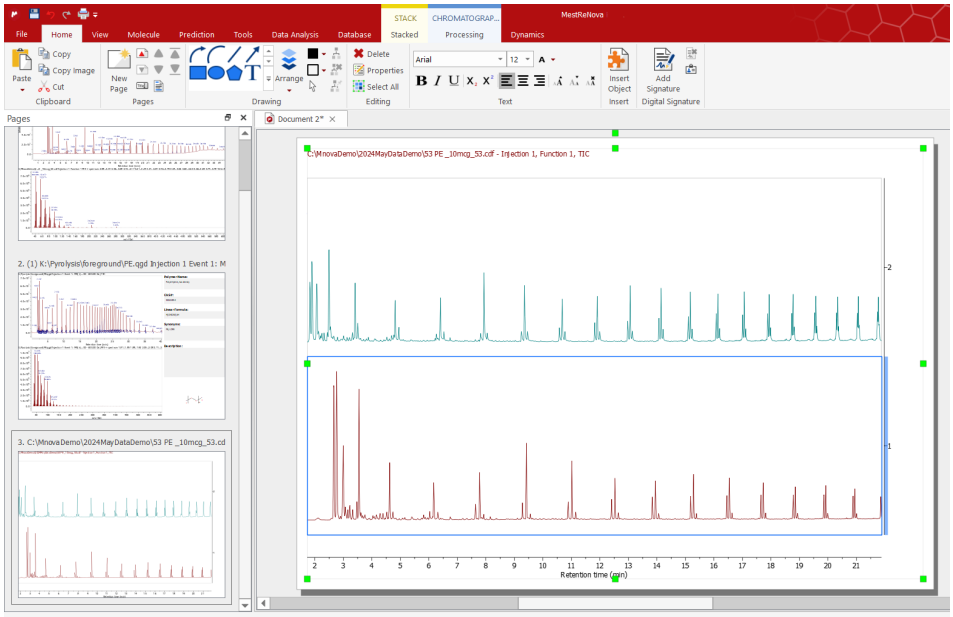
(Fill in analysis comments)



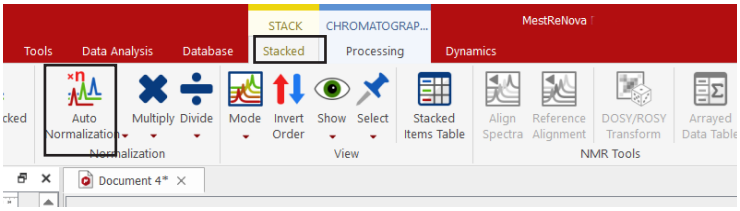
Chromatograms from the entry and the query (unknown) can be compared on the same page. This is accomplished by first pressing and holding the shift button while selecting both pages of the document in the Pages window. Then Under the CDS Ribbon and Export Chromatograms, choose "Export & Stack All Chromatograms.



A new page will open that contains both chromatograms.



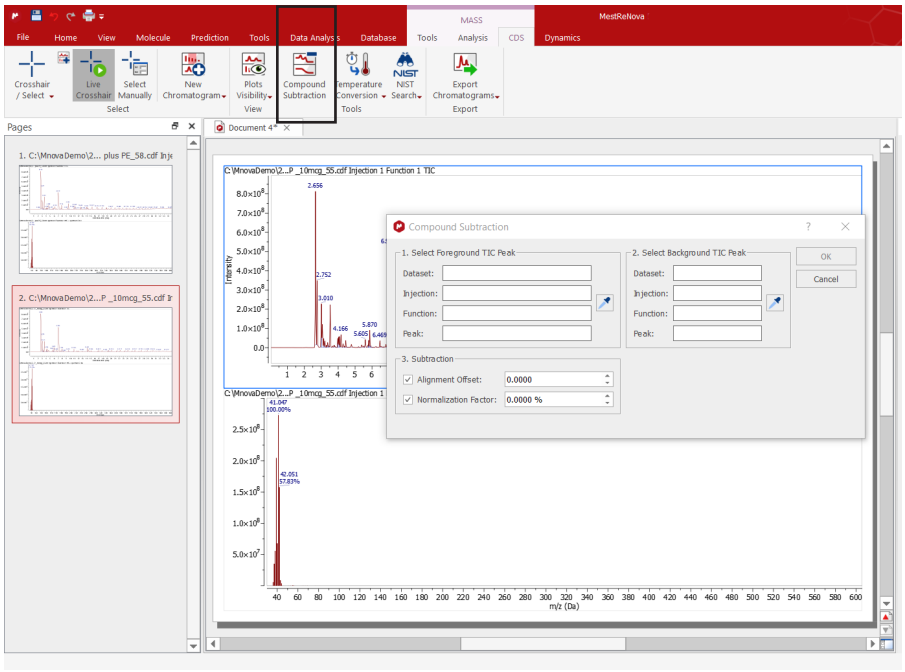
Chromatograms can be normalized by selecting the Stacked ribbon, and clicking on the Autonormalization icon.



Polymer Subtraction

In the case of a two polymer mixture, one polymer can be subtracted from the chromatogram.

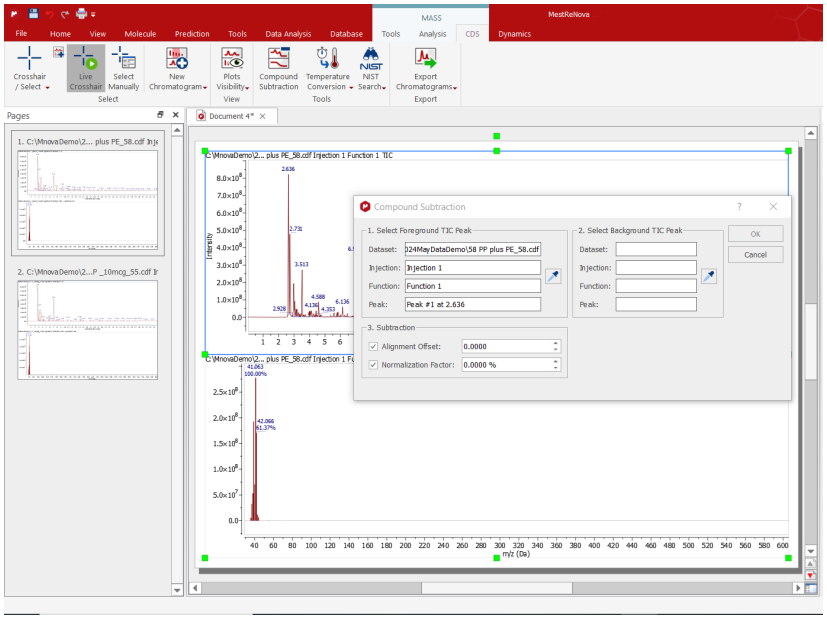
To do this, first load the mixture data. If desired, perform baseline correction on the data as described in the Baseline Correction Section. Then load the polymer data from matched database result to be subtracted. Under the CDS Ribbon, choose the “Compound Subtraction” Icon.



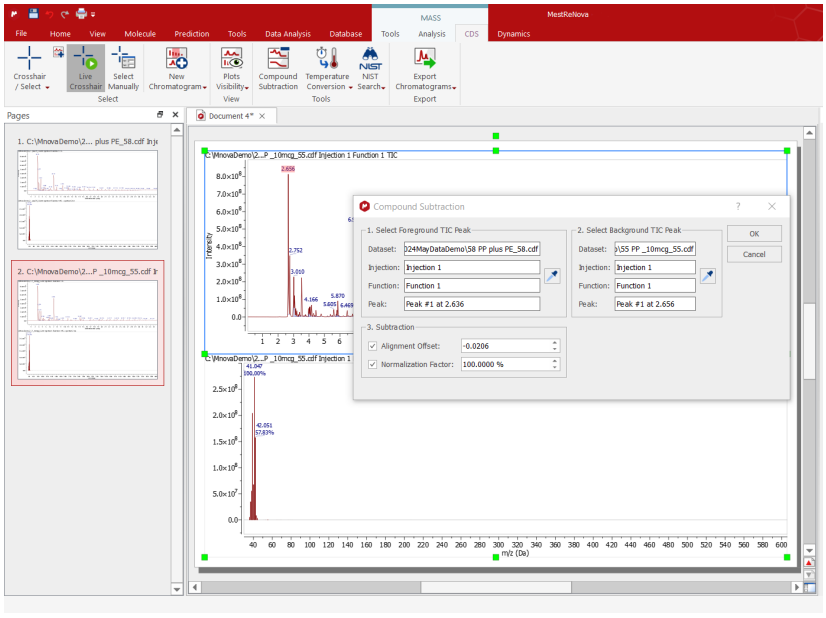
Confirm that both the Crosshair Select tool and the Zoom tool are unselected. These show up as Grey if they are selected. Click on them or press the “Esc” key to deselect them. Then you are able to use the eye-dropper to select peaks for a retention time alignment. The Foreground refers to the mixture TIC. Background refers to the single polymer TIC data.

In the Foreground box, select the page with the mixture data, which works well when choosing the most intense peak associated with the pure polymer.

\

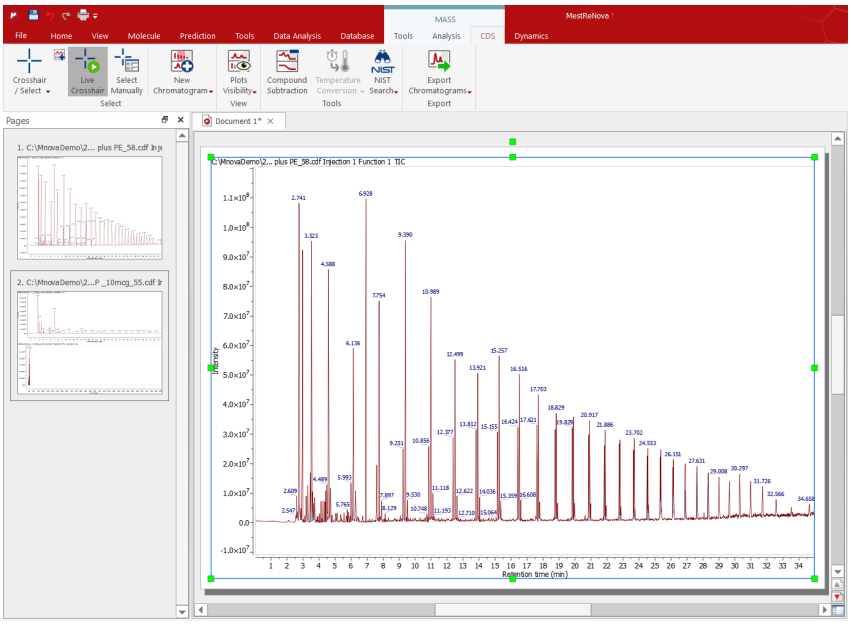


Select the Background (Polymer Standard) TIC page, depress the eyedropper in the Background TIC area, then choose the same peak in the pure polymer standard (Background).



An alignment offset and a normalization factor will be automatically calculated, but can be adjusted by the user for fine-tuning. Click OK to perform the subtraction.

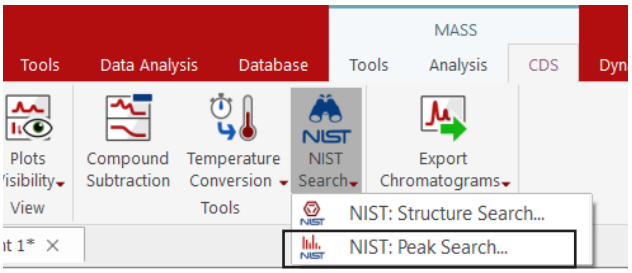
A new, Subtracted chromatogram will be calculated and available for a second search.



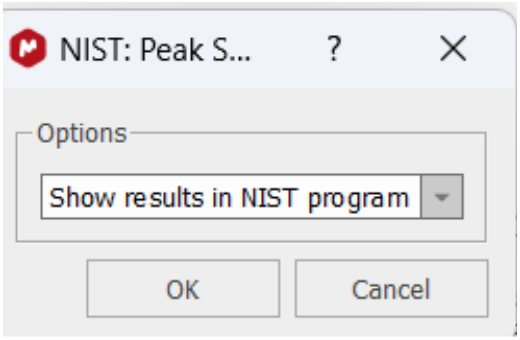
Additive Search Using NIST

The NIST library contains EI MS spectra for over hundreds of thousands small molecules. When searching additives in the pyrogram, the NIST library is an excellent tool to identify individual peaks of interest even when these peaks are not contributed by additives. The CDS additive library is designed in such a way to blend into existing NIST libraries.

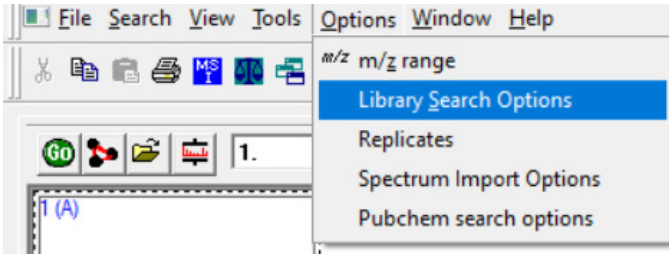
Select the peak or mass spectrum in the chromatogram to be used in a NIST peak search with the crosshair select tool under the CDS Ribbon. Then select the NIST Search Icon and choose NIST: Peak Search.



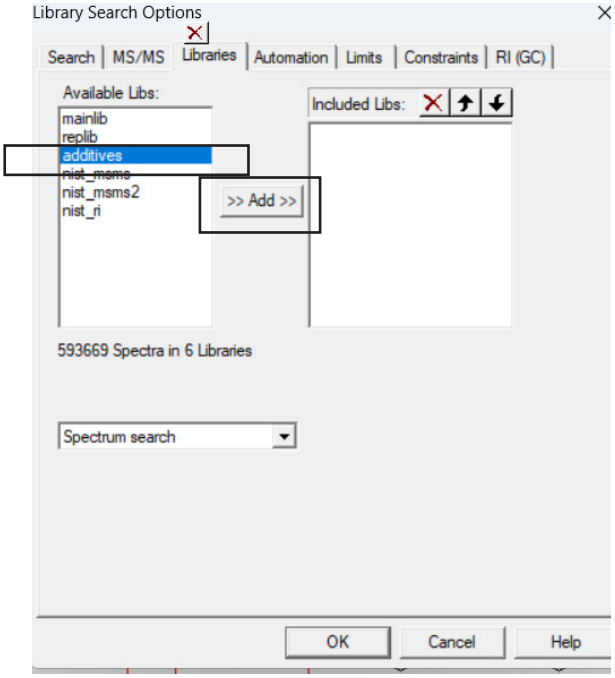
There are options available to Show Results in NIST Program or to Show Results in MestReNova (MSChrom). Choose "Show Results in NIST Program", and the NIST program will launch.



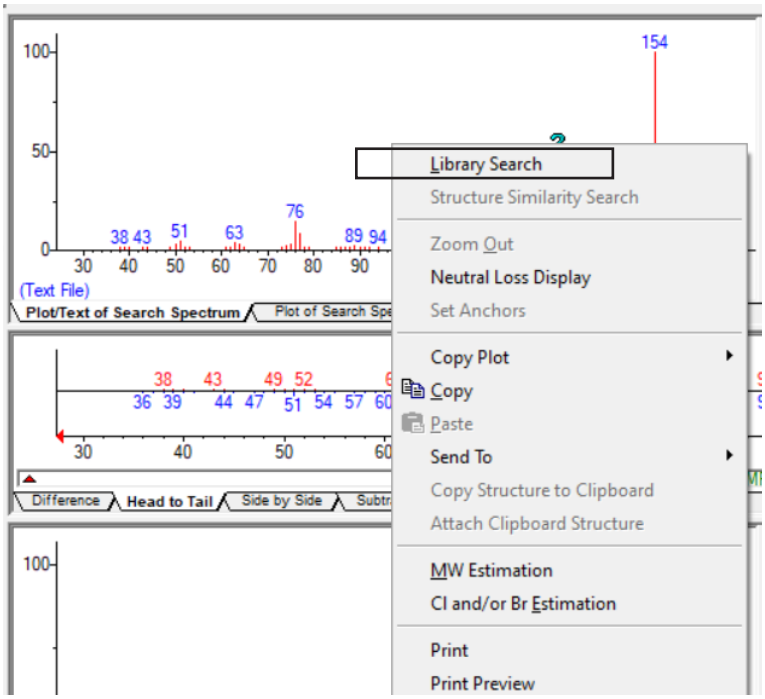
Search Results will automatically be generated with the library previously chosen. To select the desired library, choose "library search options" from the Options item in the top menu.



Select the Libraries Tab. Highlight the additives library in the left window, and press “ADD”. Press “OK”.



The search can be performed again with the correct library loaded by right-clicking on the unknown mass spectrum, and selecting “Library Search”



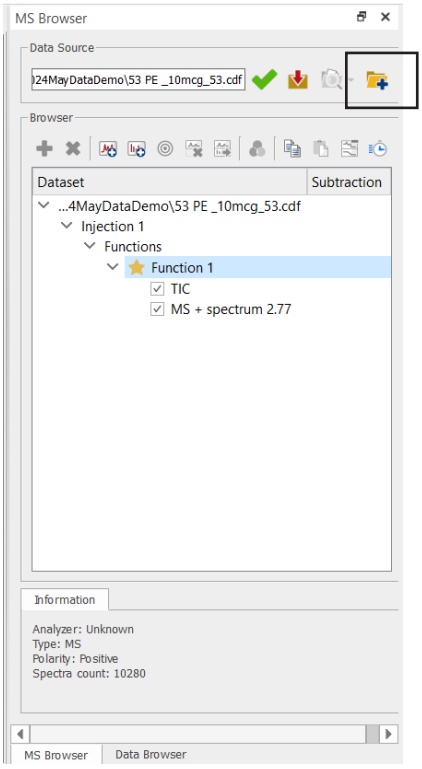
Search the EGA Database

Step 1: Temperature Conversion

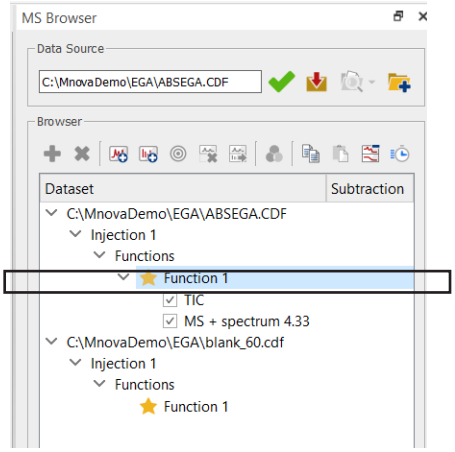
All EGA in the EGA database was collected with an initial temperature of 50°C and a final temperature of 1000°C with a ramp rate of 100°C per minute.

a. Bring the EGA data into MSChrom as described in the "Additional MSChrom Configuration" Section.

b. If baseline correction is being done, add the blank to be subtracted into the MS browser as described in (a) and (b) of "Step 1: Baseline Correction" in the "4 Steps to Search the Database" section

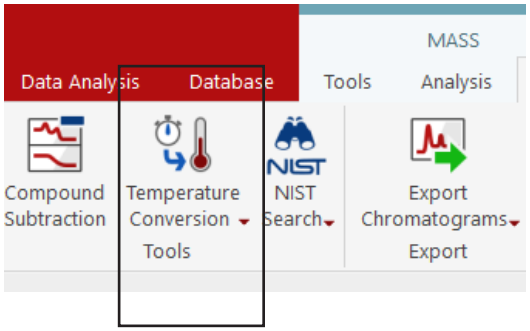


c. Each file is then converted from retention time to temperature. First select Function 1 of the sample data in the MS browser.

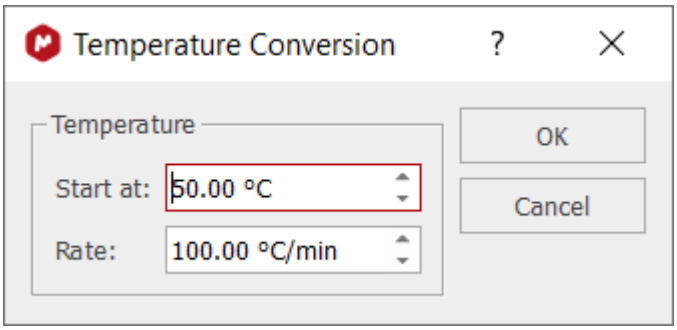


d. Convert the x-axis from time to temperature can be done pressing the "Temperature Conversion" Icon in the CDS Ribbon.

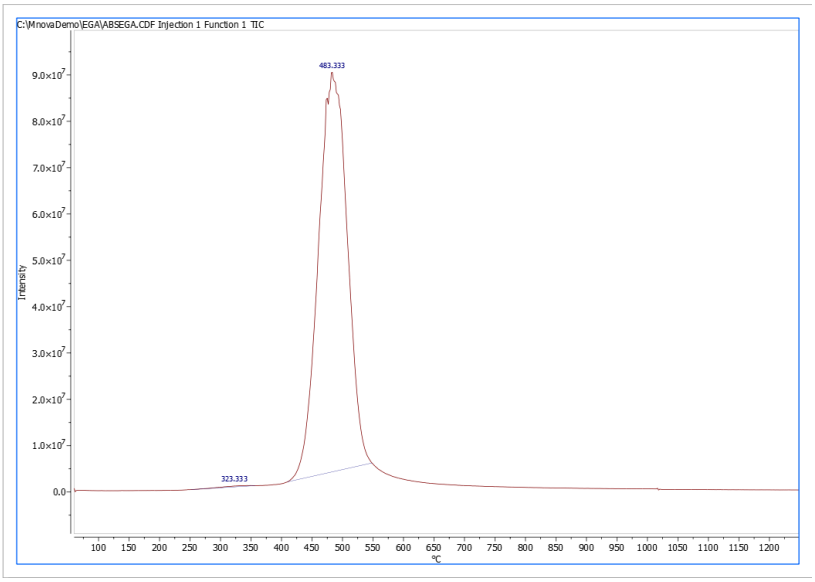
e. Convert the x-axis from time to temperature can be done pressing the "Temperature Conversion" Icon in the CDS Ribbon.



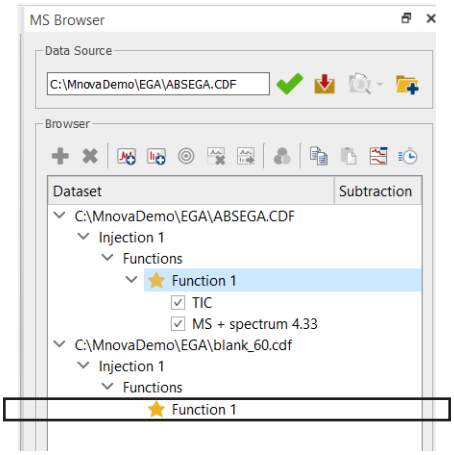
f. Enter the temperature conditions used for your EGA method and press "OK"



You will notice the conversion from time to temperature on the x-axis.

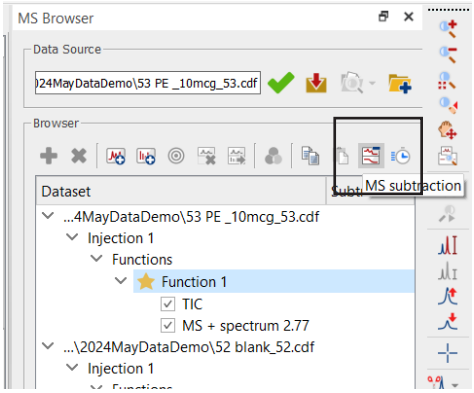


g. Transform the blank data by selecting Function 1 of this dataset and repeating (c) through (f).



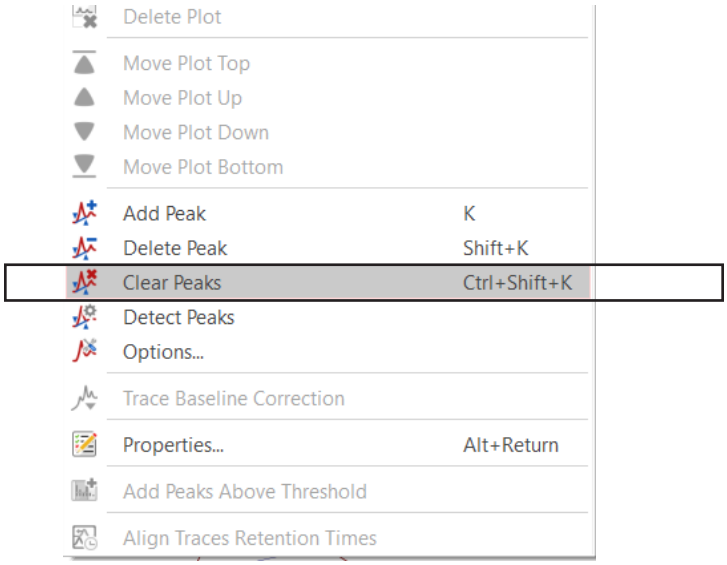
Step 2: Baseline Correction

After both EGAs are converted from time to temperature, a baseline correction can be performed by following the procedure starting from "c" "Step 1: Baseline Correction" of the "4 Steps to Search the Database" section.

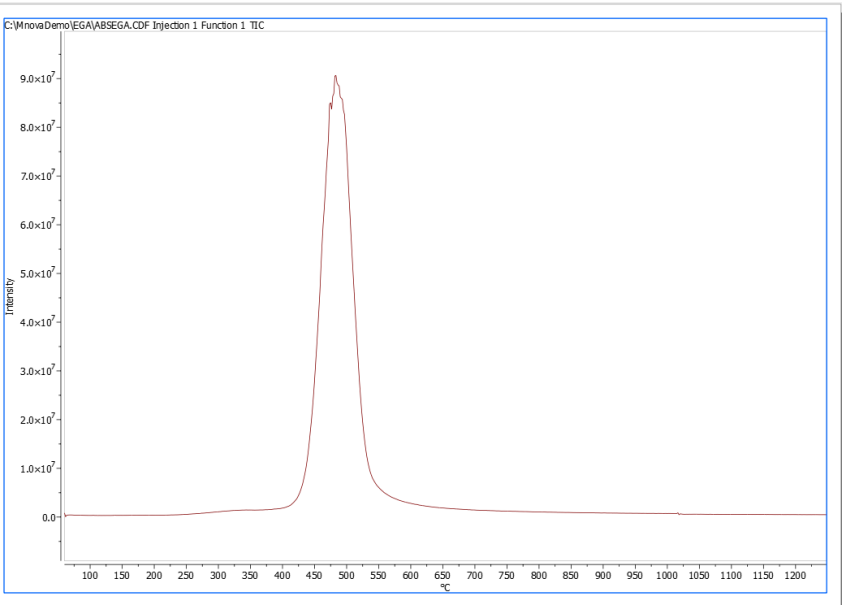


Step 3: Combine Mass Spectra for Database Search

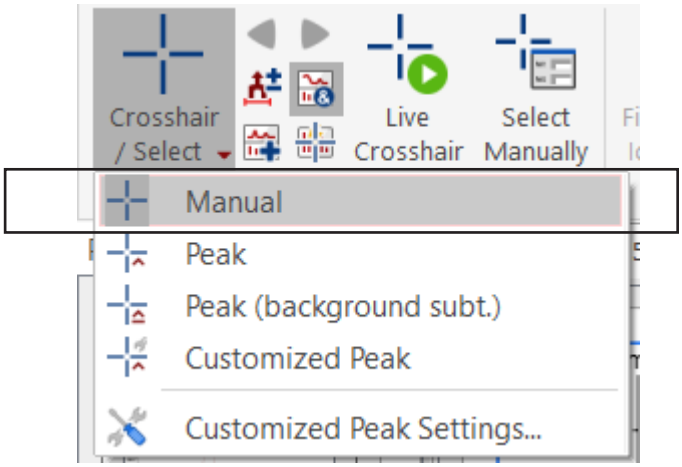
The EGA database entries have no peak integrations. Clear Peak Integrations by hovering over the EGA, right-clicking and choosing "Clear Peaks"



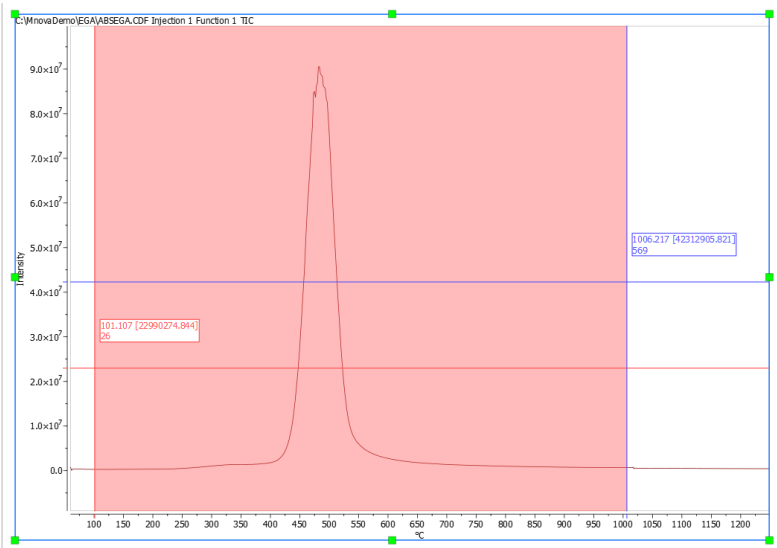
Peak integrations will be removed and the EGA will be ready to be searched against the database.



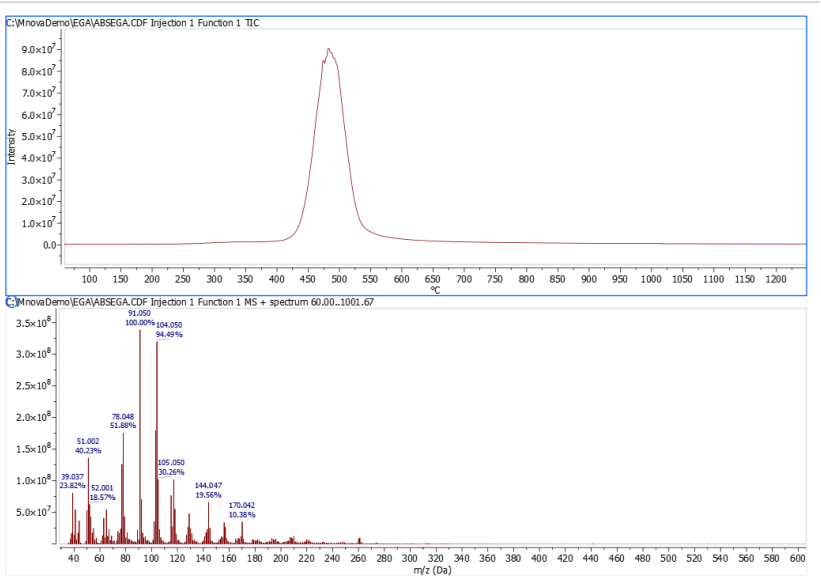
To search the database, the Mass Spectra across the EGA must be combined. With the crosshair Select tool on the CDS Ribbon, Choose "Manual"



Click, hold down and drag the mouse across the EGA to get a composite mass spectrum



A composite mass spectrum will appear below the EGA.



Step 4: Search Database

Connect to the EGA database by using the "Connect" Icon in the Database Ribbon. The EGA database is on Port 5531. The Username is Test and the Password is Database.

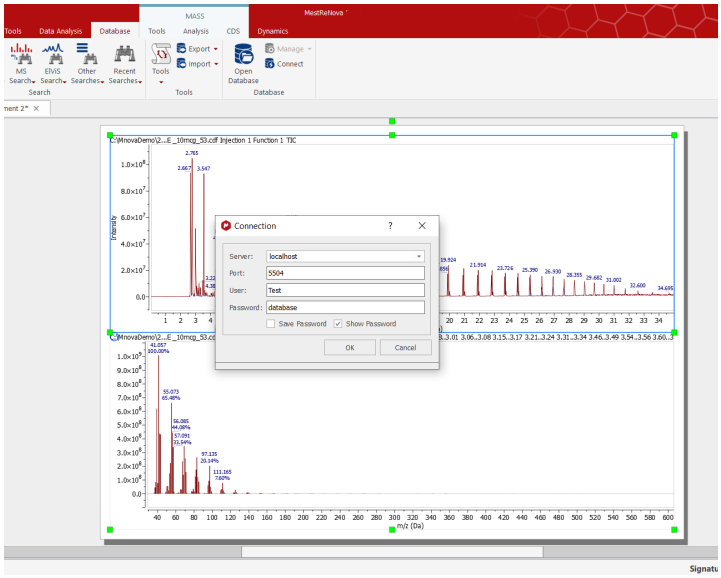
The database can be searched by hovering over the mass spectrum, right clicking and choosing MSSearch as described in "Step 3: Search Database" of the "4 Steps to Search the Pyrolysis Database" Section.

Step 5: Compare EGAs

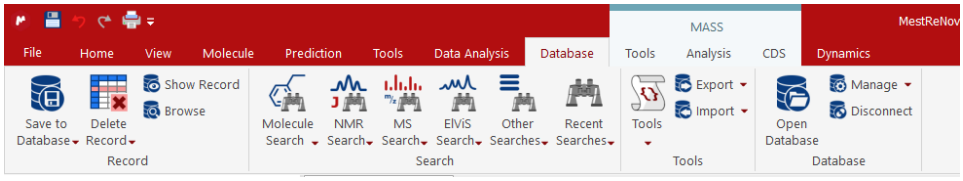
EGAs can be compared by following the procedure in"Step 4: Compare Chromatograms" of the "4 Steps to Search the Pyrolysis Database" Section.

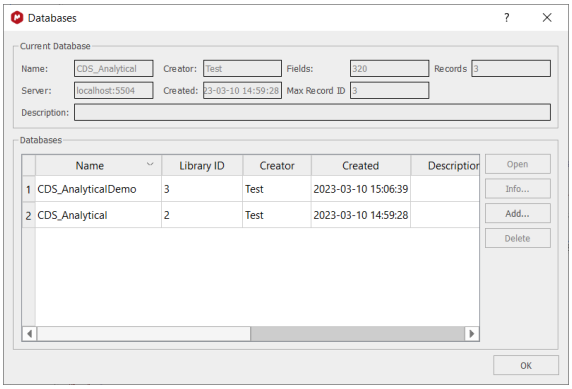
Building a Database

To create a new database, Under the Database Ribbon, select disconnect (to disconnect from any previously used databases), then select connect, under the database ribbon. Type in Port #5504, User: Test and Password: database. This is the MyData Service where personal databases can be stored.

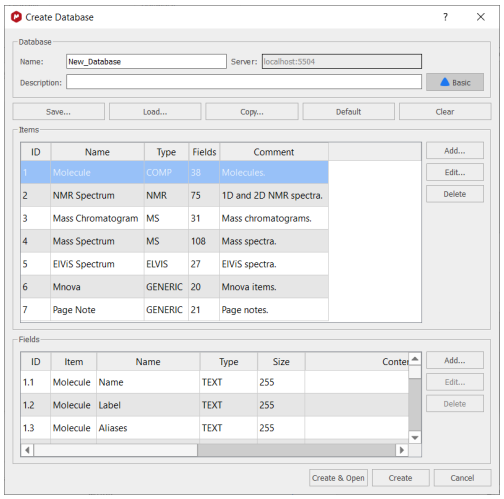


Create a database by Selecting Manage under the database ribbon. Then Choose "Add"

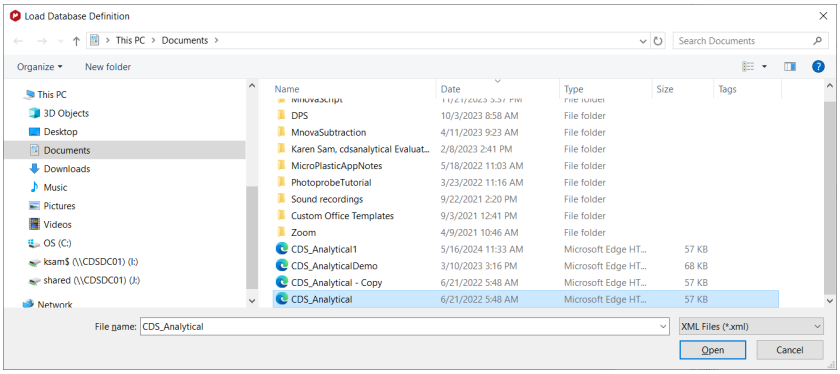




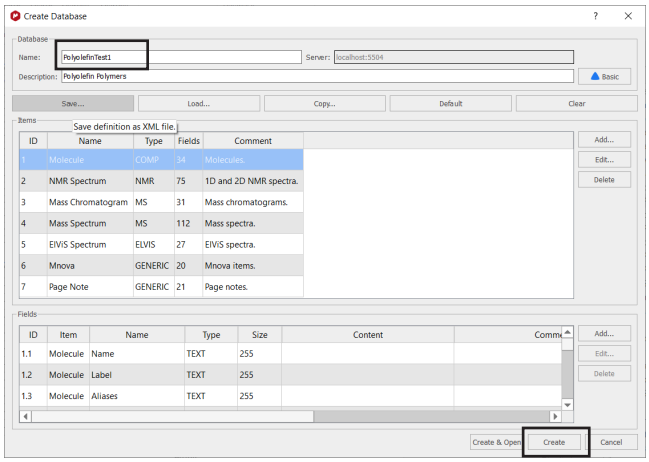
Click the advanced tab, and then press Load, to load an .xml file that will provide custom fields for the database.



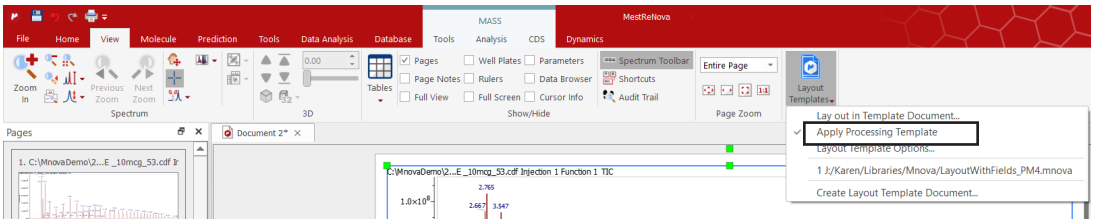
Locate and Open the CDS_Analytical.xml definition file.



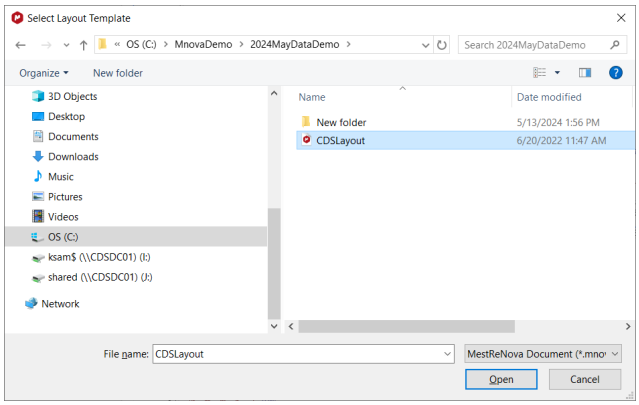
If you wish, you can rename the database, provide a description then save the new database definition. Then press create.



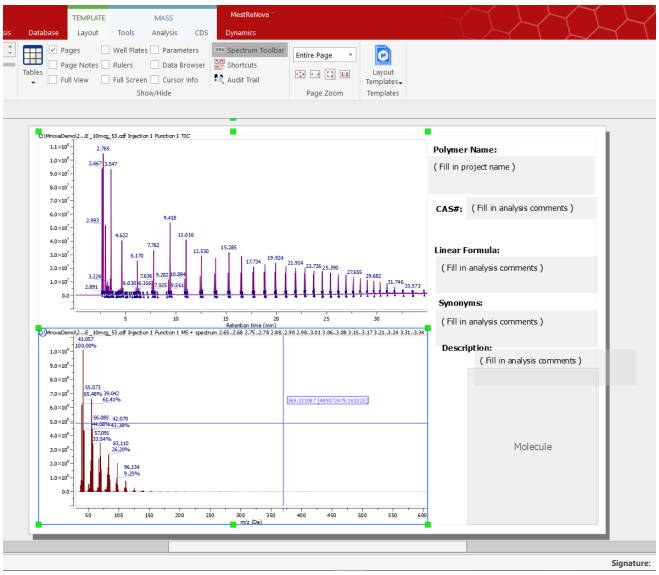
Choose Layout in Template Document, under Layout Templates in the View Ribbon.



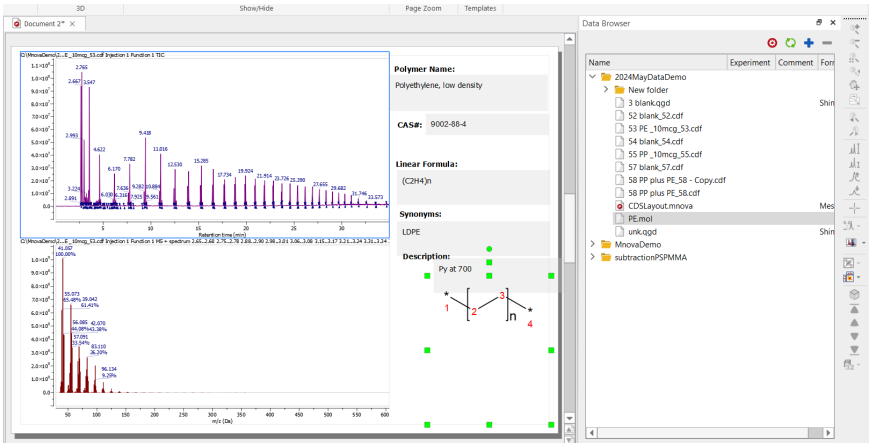
Choose CDSLayout, and open.



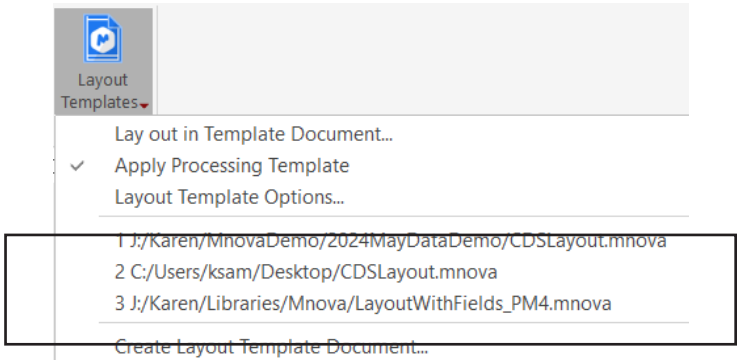
The Layout will be applied the datafile.



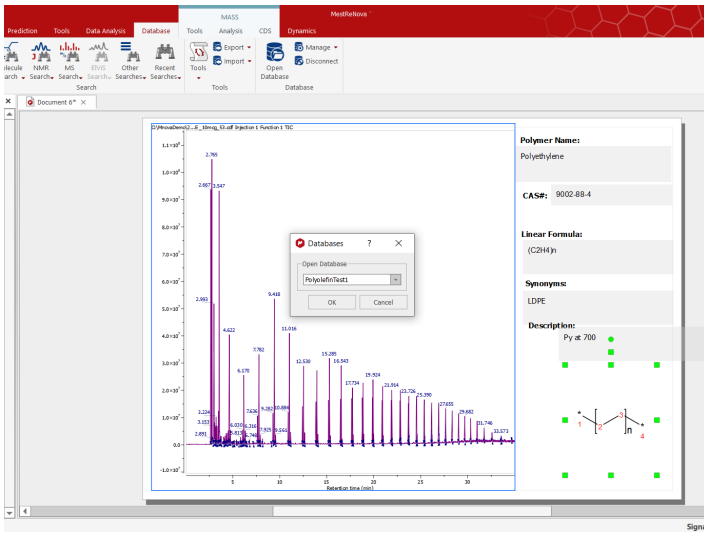
Enter information into the text boxes. A .mol file can be added to to the "Molecule" input by performing a "drag and drop" from Windows Explorer or the Data Browser



The next time you wish to apply a processing template, the layout will appear as an option under the Layout Template Icon

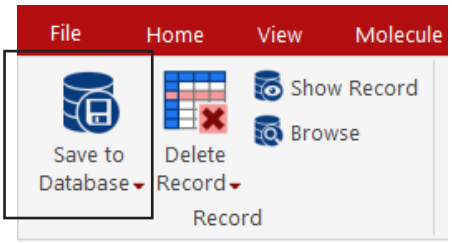


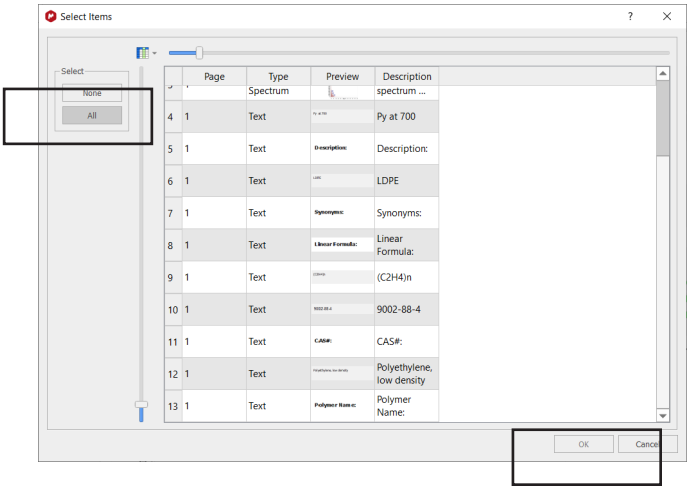
Under the Database Ribbon, Press Open Database, then choose the newly created database from the dropdown menu and press “OK”.



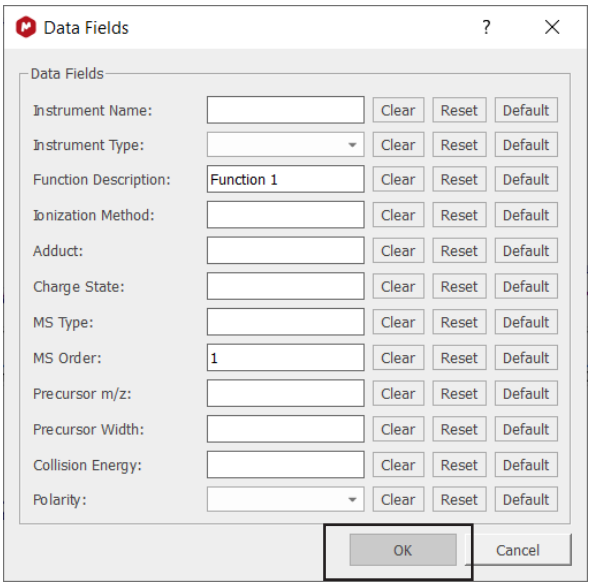
Adding to a Database

Press Save to “Database” on the Database Ribbon. Press “All”, and “OK” in the Dialog Box that opens.

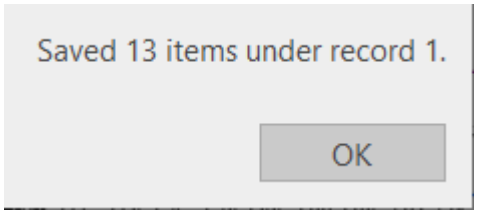




Select OK to Data Fields



An information window will notify you that your record was saved



Support

MSChrom is powerful chromatography data processing software. Additional information on its functions can be found in the areas listed below:

MSChrom Help Manual:
In MSChrom, press Fn and F2 together

The full manual in pdf form:
https://mestrelab.com/downloads/mnova/manuals/MestReNova-15.0.1_Manual.pdf

Latest information on software updates and features:
https://mestrelab.com/software/mnova-software/

Additional Resources:
https://resources.mestrelab.com/category/resources-by-product/resources-ms/

MSChrom tutorial videos:
https://www.youtube.com/playlist?list=PLEIeASG9LC-CIeY1Zs_8N2kZd59E9V-OuL