MSChrom and Database Manual



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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 identifi- cation, 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) Mno- va 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 in- cluding 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 Cur- rent and full Mass Spectra for over 600 polymers. Compatible with MSChrom search and data pro- cessing 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 soft- ware, 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.

💷 Run		×
	Type the name of a program, folder, document, or Internet resource, and Windows will open it for you.	
<u>O</u> pen:	netplwiz	~
	OK Cancel <u>B</u> rowse	

- 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).

Na	me ^	Date modified	Туре	Size
	Configuration	9/17/2024 2:37 PM	File folder	
	Manual	9/17/2024 2:37 PM	File folder	
	MnDB-CDS-Demo	7/18/2024 2:53 PM	File folder	
	MnDB-CDS-EGA	8/20/2024 4:22 PM	File folder	
	MnDB-CDS-Pyrolysis	8/20/2024 3:49 PM	File folder	
	MnDB-MyData	7/18/2024 3:10 PM	File folder	
	NIST-CDS-Additives	7/24/2024 1:48 PM	File folder	
	Tools	7/18/2024 3:10 PM	File folder	
15	MestReNova-15.1.0-37281_x64	9/17/2024 9:33 AM	Windows Installer Package	587,632 KB
0	Mnova-CDSAnalytical-1.0.0.15506.BETA	6/26/2024 2:30 PM	Microsoft Edge HTML Docume	63 KB

Description

MSChrom Manual

EGA database

DIY database

Pyrolysis database

Integration and Database Configuration files

Microplastics Py-GC-MS and EGA databas-

File/Folder

Configuration

Manual

MnDB-CDS-Demo

MnDB-CDS-EGA

Mn-DB-CDS-Pyrolysis

MnDB-MyData

NIST-CDS-Additives

Tools

Optional Items

es.

MestReNova-15.1.0-37281_x64 Installer for MSChrom software

Mnova-CDSAnalytical-1.0.0.0.15506.BETA CDSPlugin for MSChrom

NIST database of additives

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 <u>dedicated</u> 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" throu	ugh the following windows.	
	MestReNova 151 Setun - X	
	Set general installation settings for MestReNova BETA 15.1	
	Select which shortcuts will be installed	
	✓ Create a desktop shortcut	
	Create Start menu entry	
	Back Next Cancel	
Click "Next" on tl	he Custom Setup.	
	MestReNova 15.1 Setup — 🗆 🗙	
	Custom Setup Select the way you want features to be installed.	
	Click the icons in the tree below to change the way features will be installed.	
	EPR Plugin The MestReNova BETA Framework works as a container for all our specific plugins. This feature requires 20MB on your hard drive. It has 0 of 1 subfeatures selected. The subfeatures require 0KB en work before the drive drive.	
	Advanced Plugins view on your naru drive.	
	Location: C:\Program Files\Mestrelab Research S.L\MestReNova Browse	
	Reget Disk Usage Back Next Cancel	
Choose Install on	the next screen, and the software will install.	
🕼 MestReNova	- X MestReNova 15.1 Setup -	×
Ready to install MestReNova	15.1 Installing MestReNova 15.1	
Click Install to begin the installation. Cli	ick Back to review or change any of your installation	
	Status: Updating component registration	
	Back Dancel Back Next Cancel	

×



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.

MnDB-CDS-Demo	7/18/2024 2:53 PM	File folder	
MnDB-CDS-EGA	8/20/2024 4:22 PM	File folder	
MnDB-CDS-Pyrolysis	8/20/2024 3:49 PM	File folder	
	7/18/2024 3:10 PM	File folder	
NIST-CDS-Additives	7/24/2024 1:48 PM	File folder	
	7/18/2024 3:10 PM	File folder	
🚏 MestReNova-15.1.0-37281_x64	9/17/2024 9:33 AM	Windows Installer Package	587,632 KB
Mnova-CDSAnalytical-1.0.0.15506.BETA	6/26/2024 2:30 PM	Microsoft Edge HTML Docume	63 KB

This below dialog window will appear. Select "Install"

	CDS Analytical BETA		
Description:	CDS Analytical Mnova plugin		
Version:	1.0.0.15363		
Release Date	e: Wednesday, 5 June 2024		
Requires:	MestReNova (>=15.1.0.35643) MSChrom ()		
📀 Plug-i	in ready to be installed.		
Ť			
	Ins	stall	Canc
	Ins	stall	Canc
0	Information	tall ×	Canc
0	Information It is necessary to restart the application for the changes to ta	ttall X	Canc
0	Information It is necessary to restart the application for the changes to ta	ke effect.	Canc

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:

ې 🗢 💾 🧐	* 🖶 =							MASS		
File Hom	ne View	/ Mole	cule Prediction	Tools	Data Analy	rsis Databa	ase To	ools Analysis	CDS	Dynamics
_ _ 🛱			<u></u>		<u>م</u> ر	Ü,	Ä NIST	<u>_</u>		
Crosshair / Select 👻	Live Crosshair	Select Manually	New Chromatogram •	Plots Visibility 、	Compound Subtraction	Temperature Conversion 🗸	NIST Search 、	Export Chromatograms+		
	Se	elect		View		Tools		Export		

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".



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

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

My-Data

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.

	>	This PC	> Local D	isk (C:) →	NIST14 >	
This PC > Expansion (D:) >						
▲) ¢	Û	↑↓ Sort ~	🔲 View 🗸	
additives		м	SSEARCH	AMDIS32	2	

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 <u>dedicat-</u> <u>ed</u> 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."

			🕴 📑 Extract Compressed (Zipped) Folders		
	Open with MSConvertGUI Open with SeeMS	_	Select a Destination and Extract Files Files will be extracted to this folder: [C:\Users\ksam\Download\Karen Sam CDS Databases Single	B <u>r</u> owse	
	Extract All 7-Zip Pin to Start		$\ensuremath{\boxtimes}$ Show extracted files when complete		
8 2	Scan with Bitdefender Endpoint Security Tools Share Open with >				
			Extr	act Car	ncel

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

		> > MnDB-CDS	-Pyrolysis >
		🔟 🛝 Sort - 📃 View -	
Name		Name	Dat
🗋 Karen Sam Single MnDB CDS Demo v2.0.lic		Doc	7/2
🕒 Karen Sam Single MnDB CDS EGA v2.0.lic		MnClient	7/3
Karen Sam Single MnDB CDS Pyrolysis v2.0.lic		MnServer	7/3
		Services	7/3
	1	📒 Uninstaller	7/3
		.installationinformation	7/3
		1	

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".



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	TEMPLATE	Tool	MAS s Analy	S vsis	CDS	Me: Dyna	stReNova BETA		
er Recent es Searches	Tools	B Expo Impo ools	ort • ort • Data	pen abase Dat	🐻 Man 🚯 Coni	nect			
		G	Connect	ion				?	×
:			Server:	localho	ost				-
			Port:	5504					
			Password:	databa	se				
				✓ Sav	e Passv	vord 🗸	Show Passwo	ord	
							ОК	Ca	ncel
				11	near Fo	nmula	•		

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.

			Database	MSChrom	Molecule	Scripting	Drawing Tools	Python	Publication
Connection	Storage	Retrieval	Search	Scoring					
Databases	to Search	Recheval	bearen	Scoring					
Alway	s show the dat	tabase selectior	dialog						
✓ Searc Search th	h the current d e following dat	latabase (Curre tabases:	ntly: None)						
Enabled	Password	Connection							+
									1
									36
Additional	Fields to Displ	ay in Hit List —							
Item	Type Fie	eld Name							+
									×



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

references							?	×
General Plug-ins	Import	Database	Mass	e Molecule	Scripting	J Drawing Tools	Publications	
atabase Storage	a Batriaval	Search	Cooring					
Databases to Search	e Keuleval	Search	Sconing					
Always show the	database selection	i dialog						
Search the currer	nt database (Curre	ntly: None)						
Search the following	databases:							
Enabled Passwor	d Connection						+	
							/	
							×	
Additional Fields to Di	splay in Hit List							
Item Type	Field Name						!	
1 Mass Spectrum	Polymer Name						×	
				(NK (Save T Los	d Con	-al

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

Name	Experiment	Comment	Format	
> 늘 2024MayDataD	emo			
> 📁 MnovaDemo				
> 🚞 subtractionPSP	AMM			

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 0.25μ m film thickness.



Browser	[[_		
+ × 🗷	😼 💿 🐄 🖼 🐁	Ö 😫 iČ	
Dataset		Subt MS subt	tra
✓4MayDa	taDemo\53 PE _10mcg_53.cdf		
✓ Injection	on 1		
v Fu	+ Function 1		
	✓ TIC		
	MS + spectrum 2.77		
✓ …\2024Ma	ayDataDemo\52 blank_52.cdf		
• injecti	0111		
🔰 🗹 Fu	nctions		
Y Fu	nctions <hr/> <hr <="" td=""/> <td></td> <td></td>		
∨ Fu	nctions 🚖 Function 1		
Y Fu	nctions Function 1 		
Y Fu	nctions ★ Function 1		
	nctions 🚖 Function 1		
∫ ✓ Fui	nctions 🚖 Function 1		
	nctions 🔶 Function 1		
Fu	nctions 🔶 Function 1		
Information	nctions 🔶 Function 1		
Information	nctions		
Information Analyzer: Unknor Type: MS Polarity: Positive	nctions		

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".

Cel



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.

	Show Mass Browser Correlated Crosshair Synchronize Chromatograms RT Spectrum Selection Mode	Þ
14 16 16 16	Export Active Chromatogram Export All Chromatograms Export & Stack All Chromatograms Export Chromatograms	
	Extract Plot Strict Extract Plot	Ctrl+Shift+X
₹ 2 ₹ 2 ©	Hide Plot Hide Unselected Plots Show All Plots Toggle Plots Visibility	
	Delete Plot Move Plot Top Move Plot Up Move Plot Down Move Plot Bottom	
************************************	Add Peak Delete Peak Clear Peaks Detect Peaks Options	K Shift+K Ctrl+Shift+K
<i>j</i> ∿ ⊠	Trace Baseline Correction Properties	Alt+Return
	Add Peaks Above Threshold Alian Traces Retention Times	

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:





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.

Server:	localhost
Port:	5531
User:	Test
Password:	database
	✓ Save Password ✓ Show 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.

Hit	s: 1/6 Records: 1/6	Omitted: 0		None A
[Database	Recordid	Score 🖂	Polymer Name
1	CDS-Pyrolysis	11	979	Polyethylene, low density
2	CDS-Pyrolysis	8	932	Polypropylene
3	CDS-Pyrolysis	3	852	Nylon 6,6
4	CDS-Pyrolysis	2	817	Nylon 6
5	CDS-Pyrolysis	12	809	Poly[4,4'-methylenebis(phenyl isocyanate)-alt-1,4-butanediol/di(propylene glycol)/polycaprolactone]
6	CDS-Pyrolysis	5	632	Poly(methyl methacrylate)

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.

rdld <u>Score</u>	Molecule CHEMICAL STRUCTURE	Mass Chromatogram Preview	Mass Spectrum Mass Data	Recon	d	Mass Spectrue Polymer Nam
944	ČH ₃		.0 ×10 9- 0.0 100 200 300 400 50	mndb://Test@localh	ost:5532/CDS-	Poly(propylene), iso
Configure	Scores			?	×	
General		Data Selection				
Title: So	ore s	Item:		Any	-	
Icon:		Fields:				
		Name	DisplayMode	DisplayProcessor	A	
Toolbars:	Show toolbars C Default Show data references 71 113	Mass Data Mnova Versic Modified Page PageHeight PageHeight PageU PageVidth PageVidth PageVidth Proto PlotNumber Potol PlotNumber Previsew SaveID SaveID SaveID	Default Default Default Default Default Default Default Default Default Default Default Default Default Default Default Default Default Default		V	

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.



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.





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

То	ols Data Ana	alysis Databa	STACH ase Stacke	CHROM	ATOGRAP essing	Dynan	N nics	destReNova		
: cked	Auto	Multiply Divide	Mode Inver	t Show Se	lect Stac	ked Table	Align Spectra	Reference Alignment	DOSY/ROSY Transform	Arrayed Data Table
	Norrha		View				NMR Tools			
5	× ODocur	ment 4* ×								

Polymer Subtraction

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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 sub-traction.





Additive Search Using NIST

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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.

VIST: Peak S ? X
Options Show results in NIST program
OK Cancel
Leparation (D) × + × Nort M Sector L2- Joint, Present Default - Index 2.9 (Sector Parater Default - Index 2.9 (Sector Parat
100 100
is Made // PMade/h PMad/h PMade/h PMad/h PMade/h PMade
15 ad 200 475 0.28 Deerof influide

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".

Library Search Options	Automation Limits Constraints RL(GC)
Available Libs: mainlib replib additives nist_msms2 nist_ri	Included Libs: ★★
593669 Spectra in 6 Librarie Spectrum search	es T

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

Subtractio
Subtractic

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.



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



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.



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



Step 2: Baseline Correction

Step 3: Combine Mass Spectra for Database Search 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





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"

Inc None Colle Prediction Tools Database Tools Database Save to Database + Record Show Record Image: Show Record <td< th=""><th>nage 👻</th></td<>	nage 👻
Save to Delete Delete Show Record Database Record NMR MS Elvis Other Record Tools Database Database Record Search Search Search Search Search Search Tools Database Database Record Center Center Feddate Search Search Search Search Search Tools Database Database Center Center Feddate Search Search Search Search Tools Database Database Center Center Search Tools Database Database Database Tools Database <t< th=""><th>nage 🝷</th></t<>	nage 🝷
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Record Search Tools Database Current Database ? X Current Database ? X Description:	
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Current Database Current Database Name: CDS_Analytical Demo 3 Test 2023-03-10 15:06:39 Cost 2 CDS_Analytical 2 Test 2023-03-10 15:06:39 Cost 2 CDS_Analytical 2 Test 2023-03-10 15:06:39 Add	
Current Database Name: CDS_Analytical Cre ator: Test. 3200 Record S Sever: Becords Becords<	
Name: CDS_Analytical Creator: Test 320 Record ID Server: localhost:5564 Created: [2:43:10:14:159:28] Max Record ID 3 Description:	
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Delete	
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Click the advanced tab, and then press Load, to load an .xml file that will provide custom fields for the database.

Dataha									
Name:	New_D	atabase			Serve	r: localhost:5	504		
Descrip	tion:								🔺 Basic
	Save		Load		Co	ру		Default	Clear
Items-									
ID	N	ame	Туре	Fields		Comment			Add
									Edit
2	NMR Spec	trum	NMR	75	1D and	2D NMR spe	ectra.		Delete
3	Mass Chro	matogram	MS	31	Mass d	hromatogram	15.		
4	Mass Spec	trum	MS	108	Mass s	Mass spectra.			
5	EIViS Spec	trum	ELVIS	27	EIViS s	ElViS spectra.			
6	Mnova		GENERIC	20	Mnova	Mnova items.			
7	Page Note	9	GENERIC	21	Page n	otes.			
Fields-									
ID	Item	N	lame		Туре	Size		Conter	Add
1.1	Molecule	Name		TEX	π	255			Edit
1.2	Molecule	Label		TEX	π	255			Delete
1.3	Molecule	Aliases		TEX	т	255			
4									

Locate and Open the CDS_Analytical.xml definition file.

→ ✓ ↑ 🖺 > This PC > Documents >				~	Ü	Search Documer	nts	
Organize • New folder						8		
🧏 This PC	^	Name	Date	Type	Size	Tags		
3D Objects		DPS	10/3/2023 8:58 AM	File folder				
Desktop		MnovaSubtraction	4/11/2023 9:23 AM	File folder				
Documents		📜 Karen Sam, cdsanalytical Evaluat	2/8/2023 2:41 PM	File folder				
Downloads		MicroPlasticAppNotes	5/18/2022 11:03 AM	File folder				
Music		PhotoprobeTutorial	3/23/2022 11:16 AM	File folder				
Pictures		Sound recordings	9/22/2021 2:20 PM	File folder				
Videos		Custom Office Templates	9/3/2021 12:41 PM	File folder				
		Zoom	4/9/2021 10:46 AM	File folder				
C 03 (C.)		CDS_Analytical1	5/16/2024 11:33 AM	Microsoft Edge HT		57 KB		
🛫 ksam\$ (\\CDSDC01) (I:)		CDS_AnalyticalDemo	3/10/2023 3:16 PM	Microsoft Edge HT		68 KB		
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Network	~	CDS_Analytical	6/21/2022 5:48 AM	Microsoft Edge HT		57 KB		
File events CDC Arelation					_	NA 10 10 10 10		

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

Jame:	Pakalw	finTert1		_	_		Separa localbort-5504			
vanie.	Polyole	minesti					Server. Incariosc.5304			
Descrip	tion: Polyole	fin Polymers] [Basic
	Save			Load	ł		Сору	Default	Clea	r
lems	Sav	e definition	as XML file	a .						
ID	Na	ame	Туре	Fields		Comment				Add
										Edit
2	NMR Spec	trum	NMR	75	1D and	2D NMR spectr	а.			Delete
3	Mass Chro	matogram	MS	31	Mass d	hromatograms.				
4	Mass Spec	trum	MS	112	Mass s	pectra.				
5	EIViS Spec	trum	ELVIS	27	EIViS s	pectra.				
6	Mnova		GENERIC	20	Mnova	items.				
7	Page Note		GENERIC	21	Page n	otes.				
ields										
ID	Item	N	ame		Туре	Size	Content		Comme	Add
1.1	Molecule	Name		TEX	т	255				Edit
1.2	Molecule	Label		TEX	т	255				Delete
1.3	Molecule	Aliases		TEX	т	255				
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Choose Layout in Template Document, under Layout Templates in the View Ribbon.

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Pages 5 × O Do	cument 2* ×	aDemo\2E_10mcg_53.cdf Injection 1 Function 1 T		Apply Processing Template Layout remplate Options Lyout remplate Options L/Karen/Libraries/Mnova/LayoutWithFields_PM4.mnova
	1.0>	2.765 10 ⁸ 2.667 3.547		Create Layout Template Document

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		Page	Type	Preview	Description	
None	ר ר		Spectrum	L	spectrum	
All	4	1	Text	Py 4788	Py at 700	
	5	1	Text	Description	Description:	
	6	1	Text	LINE	LDPE	
	7	1	Text	Synonyms:	Synonyms:	
	8	1	Text	Linear Formula:	Linear Formula:	
	9	1	Text	(Tash	(C2H4)n	
	10	1	Text	N002-88-4	9002-88-4	
	11	1	Text	CAS#:	CAS#:	
	12	1	Text	Projettylens, kar denety	Polyethylene, low density	
	13	1	Text	Polymer Name:	Polymer Name:	

Select OK to Data Fields

🕑 Data Fields				?	×
Data Fields					
Instrument Name:			Clear	Reset	Default
Instrument Type:		*	Clear	Reset	Default
Function Description:	Function 1		Clear	Reset	Default
Ionization Method:			Clear	Reset	Default
Adduct:			Clear	Reset	Default
Charge State:			Clear	Reset	Default
MS Type:			Clear	Reset	Default
MS Order:	1		Clear	Reset	Default
Precursor m/z:			Clear	Reset	Default
Precursor Width:			Clear	Reset	Default
Collision Energy:			Clear	Reset	Default
Polarity:		Ŧ	Clear	Reset	Default
			ОК		Cancel

An information window will notify you that your record was saved

Saved 13 items u	nder record 1.
	ОК

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=PLEleASG9LC-CleY1Zs_8N2kZd59E9V-OuL