

"Converting NIST User Library to Wiley User Library"

James Little Mass Spec Interpretation Services

Handouts for Videos: Website: "Little Mass Spec and Sailing" <u>https://littlemsandsailing.wordpress.com</u>

Note: In-depth training videos/handouts on this new mass spec software on my website!

Creating NIST Libraries to Wiley Libraries

► NIST libraries cannot be searched by KnowItAll

➤Wiley libraries cannot be searched by NIST Search

However, NIST user libraries can be converted to Wiley Format

NIST Commercial libraries cannot be converted

➢ Possibly Wiley specialty libraries can be converted, but not attempted

First Export the NIST Library

► Use the NIST utility, Lib2NIST distributed with the NIST software

Find the library in NIST Lib Format

Export the library of interest in SDF format

The SDF format includes structure, ion, ion intensities, and various other fields
 It is an ASCII file format and can be opened and viewed with Windows Notepad

Convert MS Libraries or Da	tafiles to NIST o –		MS Librarios or Datafila		×
Select Input MS Library or D	atafile	Convert	IVIS LIDIAILES OF Dataille		~
Drives: Path:		NIST Library	C:\NIST20\MSSEARCH		
[□ [-C-]	RCH\	Output	C:\NIST20\MSSEARCH		
Image: DD2014 Image: DD2020 Image: DD2021 Image: DD2022 Image: DD2022 <td< td=""><td>Image: glycolate monoesters eastman Image: glycolate monoesters eastman</td><td>Im_l Input Librarie Im_r Input Librarie Im_r C:\NIST20\N Im_r Input Librarie Im_r C:\NIST20\N Im_r Input Librarie Im_r C:\NIST20\N Im_r Input Librarie Im_r Inp</td><td>rs or Text Files</td><td>NIST MS User Libraries</td><td></td></td<>	Image: glycolate monoesters eastman Image: glycolate monoesters eastman	Im_l Input Librarie Im_r Input Librarie Im_r C:\NIST20\N Im_r Input Librarie Im_r C:\NIST20\N Im_r Input Librarie Im_r C:\NIST20\N Im_r Input Librarie Im_r Inp	rs or Text Files	NIST MS User Libraries	
HP Lib (*.L), Text (*.SDF, *.MSP), NIST	Lib(*.*) Open	Cancel	Use subset	Output Format	•
Add Input Libraries/Files	Convert	Add Input Li	praries/Files Conv	vert Exit	

Import the SDF File Into Wiley KnowItAll Minelt Program

➢Go to Minelt and File/Create New Database option

➤Assign Database Name

Assign Database Abbreviation up to 7 letters

The latter field is the one displayed with the search results

Create on local system, put in a folder external to Wiley software

➤Then import the SDF file

New Database Creation	×	File Edit View Database Hit I	ist MS Tools Windo
Create on local system Create on network		New Database Open Database Open Hit List	Ctrl+N Ctrl+O
Database File Name:	Browse	Close Close All	Ctrl+W/F4
Database Abbreviation: jitest Version: 1.00 First ID: 1		Batch Import Import Attachment(s) Export Save Hit List As Edit Report Templates Print	Ctrl+I , Ctrl+P
Brief Copyright	ОК	Preferences Define Command Line Parame	ters
	Cancel	Recent Files Exit	, Alt+F4

Map the Fields in NIST Library Into the Wiley Format

In intermediate window, remember to select "Add Implicit Hydrogens"
Map the SDF File Property to ones shown for the SDBX file
Can add user properties, but *best* to match ones in their list
Do not have to import all fields if thought not useful
See tips in video on how to effectively use the interface

	zing SDF File		
Encoding:	<default></default>	~	
Text Sample:	COMMENT: component number 1 in jltest library EXACT MASS: 155.050177 FORMULA: C8H10CIN ID: 1 INCHIKEY: VNTUPELUDLYWRD-UHFFFAOYSA-N MASS SPECTRAL PEAKS: 39 127	•	
Records to i	mport) Records:		
] Import all Auto-com	data into the current database record pute properties during import it bydrogens		
☐ Import all ☐ Auto-com ☐ Add implic The file was a	data into the current database record pute properties during import it hydrogens malyzed successfully (5 records read).	-	

ep 2: Mapping Properties	and Fields
Map SDF to available SDB	X/SDB properties and fields
SDF file	SDBX file
COMMENT	Gas Chromatogram
EXACT MASS	MOA
FORMULA	MOACONF
ID	Modulus
INCHIKEY	Mold Shrinkage
MASS SPECTRAL PEAKS	Mole Percent Hydrolyzed
MW	Molecular Weight
NAME	MRDD mg
NUM PEAKS	MRDD mmol
	MS Parameters
Use to link existing rec	cords MS Peak Lists
	MS Quad Temperature
Suggest Sugg	Jest All MS Source Temperature
	MS Threshold
Examples found in this SI	DF file for the MSD Transfer Line Temperature
39 127	MSDS
	Mutagenicity
42 14	Mutagenicity in Salmonella
20.64	Mutagenicity Predicted
38 64	Mutagenicity Predicted Confidence
	Neurotoxicity
	Neurotoxicity Predicted
< B	ack Nex Neurotoxicity Predicted Confidence
	Neutralization Number
	NIST ID
	NMR Offset
	NMR Reference Standard
	NMR Spectrometer Frequency

"Store as Numeric Value" Issue

Make sure "Store as Numeric Value is **not clicked**, it will cause problems when the library is created

Before completing Step 2 and saying "Next", once again make this radio button is not selected!



Mapping Values

NIST Field Name	Wiley Field Name		
COMMENT	COMMENT		
EXACT MASS	EXACT MASS		
FORMULA	Formula		
ID	Record ID		
INCHIKEY	InChiKey		
MASS SPECTRAL PEAKS	MS Peak Lists		
MW	Nominal Mass		
NAME	Name		
NUM Peaks	NUM PEAKS		

Final Steps

Make sure "Store as Numeric Radio Button" *not* selected

➤Take option to compact database

➤Use standard compaction options

➤Good to check library, see method in video

MoNA EI Libraries

▶18,886 free El spectra

➤ Quality is reasonable, but do find errors

> Derivatives are shown as their underivatized structure in search results

MassBank of North America, <u>click here</u> for website

>I have created the MoNA EI library in both NIST and Wiley Formats

<u>Click link</u> for downloading MoNA EI library in Wiley Format

<u>Click Link</u> for downloading MoNA EI library in NIST format