KnowItAll Mass Spectrometry Training

Vendor Neutral Data Processing Solution for Spectral Analyses

WILEY

KnowItAll™

"Converting NIST User Library to Wiley User Library"

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

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

Link to Training

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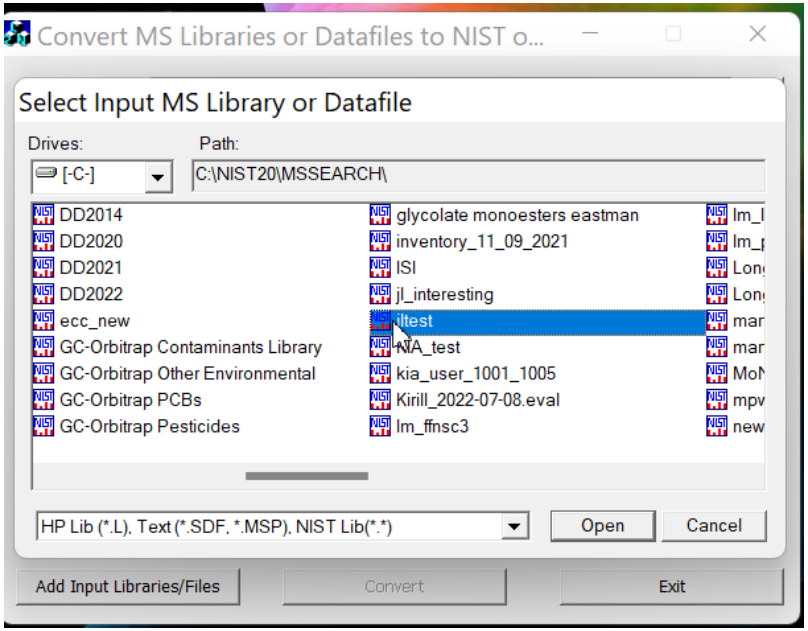
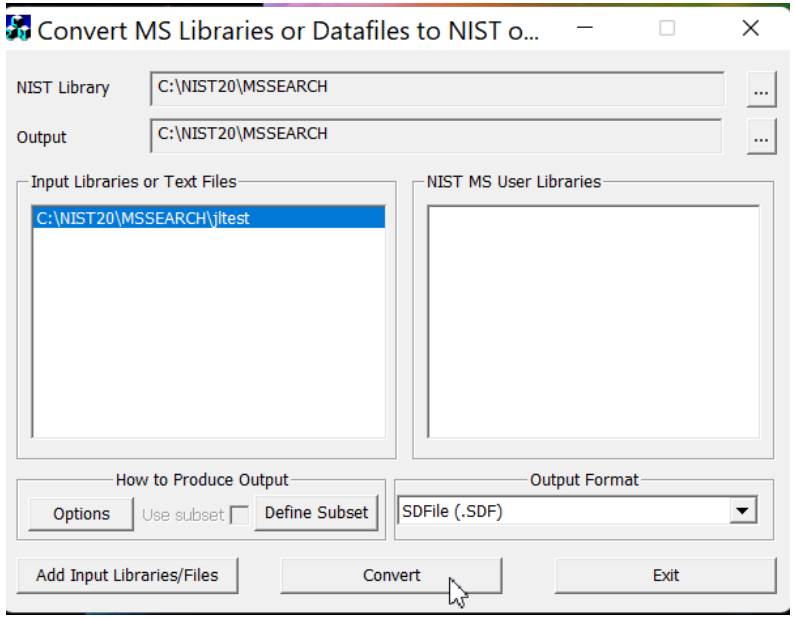
Creating NIST Libraries to Wiley Libraries

- 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

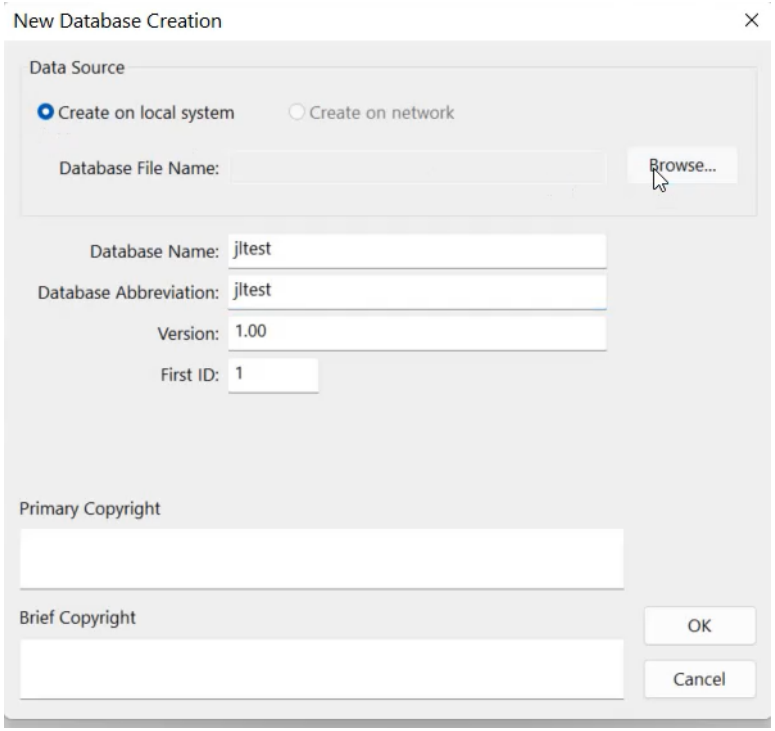
- Use the NIST utility, Lib2NIST distributed with the NIST software
- Find the library in NIST Lib Format
- Export the library of interest in SDF format
- The SDF format includes structure, ion, ion intensities, and various other fields
- It is an ASCII file format and can be opened and viewed with Windows Notepad

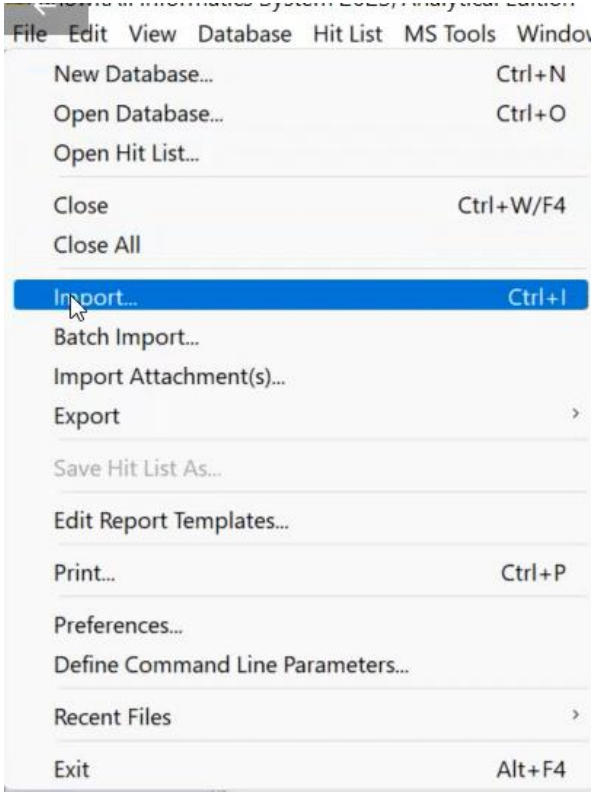




Import the SDF File Into Wiley KnowItAll MineIt Program

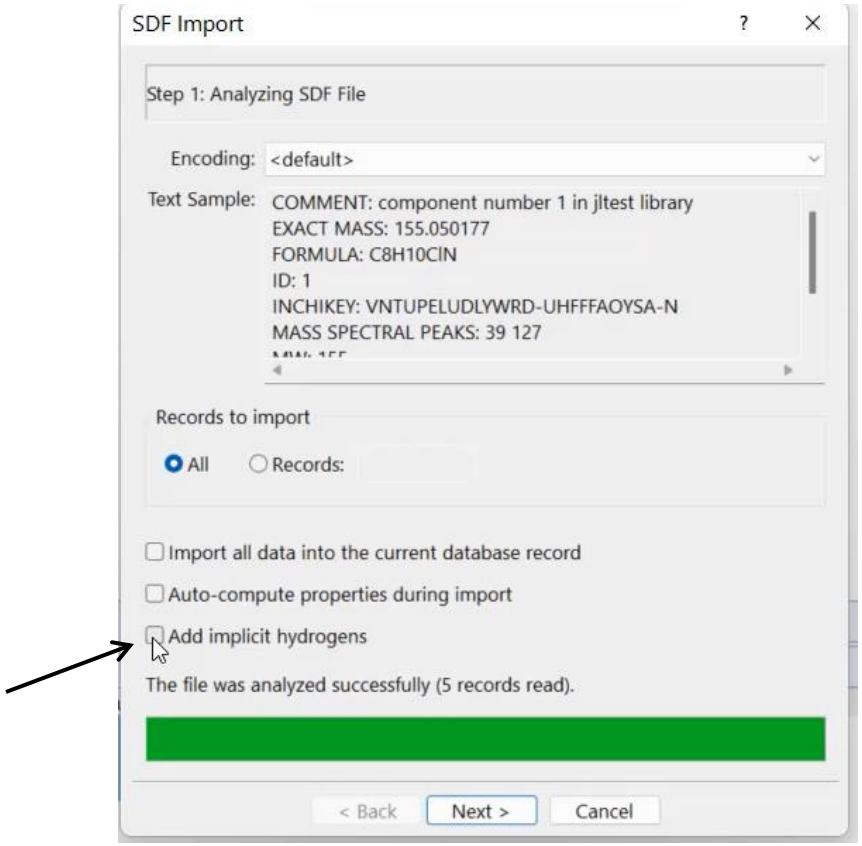
- Go to MineIt and File/Create New Database option
- Assign Database Name
- Assign Database Abbreviation up to 7 letters
- The latter field is the one displayed with the search results
- Create on local system, put in a folder external to Wiley software
- Then import the SDF file

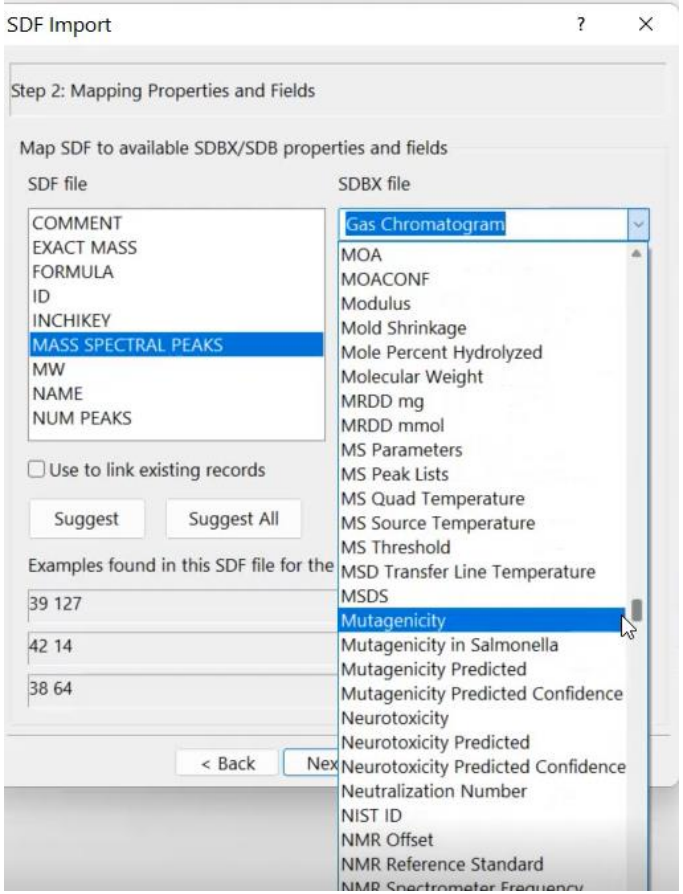




Map the Fields in NIST Library Into the Wiley Format

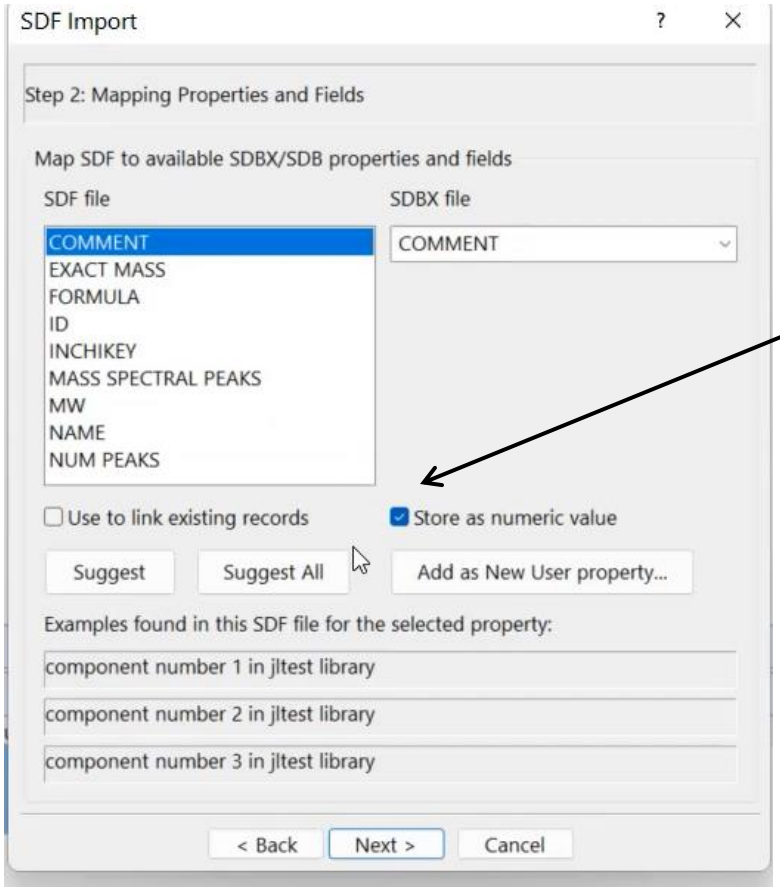
- In intermediate window, remember to select “Add Implicit Hydrogens”
- Map the SDF File Property to ones shown for the SDBX file
- Can add user properties, but ***best*** to match ones in their list
- Do not have to import all fields if thought not useful
- See tips in video on how to effectively use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





“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!



Make sure this radio button ***not*** selected for any fields, will cause problems creating library, check all fields created!

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 EI spectra
- Quality is reasonable, but do find errors
- Derivatives are shown as their underivatized structure in search results
- MassBank of North America, *click here* for website
- I have created the MoNA EI library in both NIST and Wiley Formats
- *Click link* for downloading MoNA EI library in Wiley Format
- *Click Link* for downloading MoNA EI library in NIST format