

KnowItAll Mass Spectrometry Training

*Vendor Neutral Data Processing
Solution for Spectral Analyses*

WILEY



KnowItAll™

“Transferring Spectra from KnowItAll to NIST Search”

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Mass Spec Interpretation Services

Handouts for Videos:

Website: Little Mass Spec and Sailing

<https://littlemsandsailing.wordpress.com>

NOTE: Series of other training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

Reasons for Transferring Spectra from KnowItAll to NIST Search

Reasons for Transferring

- A library is only present in NIST format but not KnowItAll Format
- NIST sequential searches very useful in querying libraries
- NIST MS Interpreter for correlating substructures to observed ions
- Compare KnowItAll search results to those found by related searches in NIST
- Use ProcessIt to manually obtain spectra, and send to NIST search
- AMDIS not as easy as ProcessIt in manual mode to obtain spectra for NIST search

Video Course on Using NIST Search

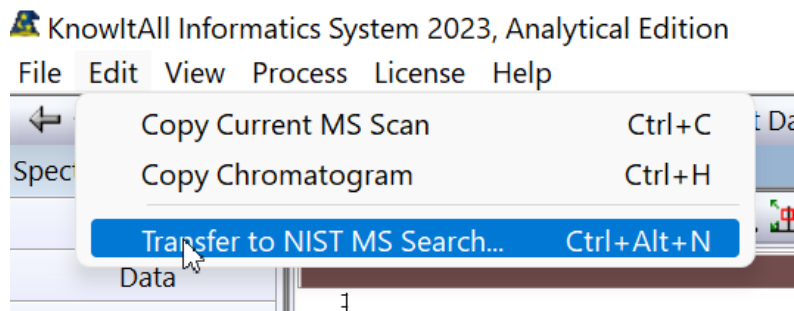
<https://littlemsandsailing.wordpress.com/2020/08/17/ms-master-class/>

NOTE: Video available on my personal website to convert NIST user libraries to Wiley Format

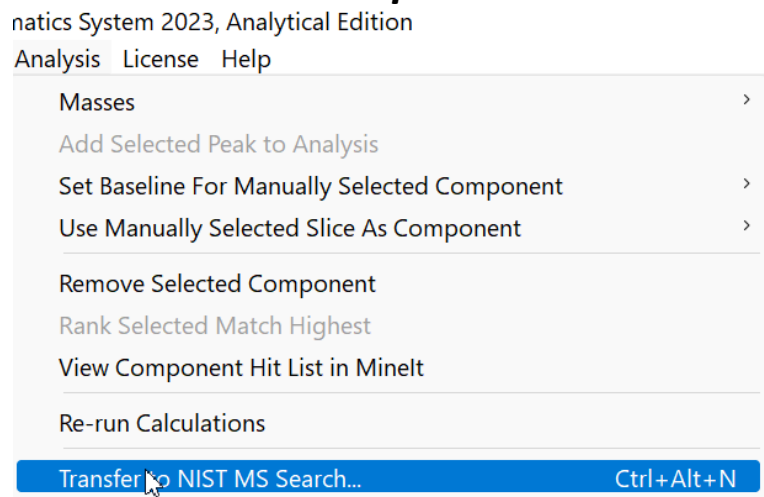
Can Transfer to NIST Easily from KnowItAll in Three Programs

- ProcessIT, SearchIT, and MS Expert
- In ProcessIt, left click on spectrum in bottom window, then edit pull down menu
- In SearchIt, also Edit pull down menu
- In MS Expert, select spectrum of interest in Component window, then Analysis pull down menu
- All use key sequence Ctrl+Alt+N key sequence
- Easily return to KnowItAll with “Switch to Caller” arrow in NIST Search

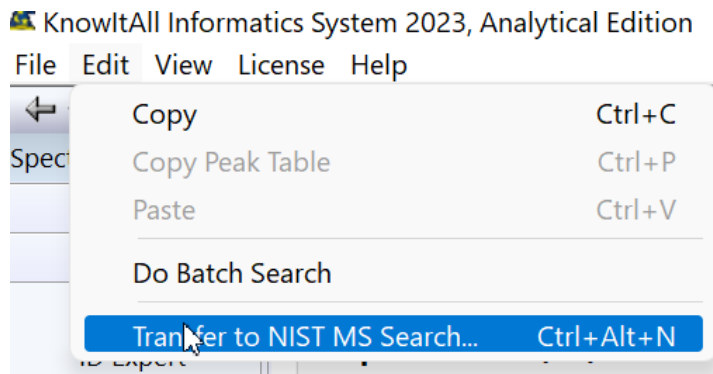
ProcessIt



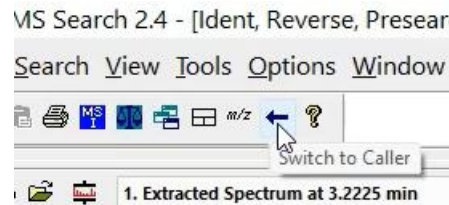
MS Expert



SearchIt



NIST “Switch to Caller” Button



Can Transfer to KnowItAll from NIST Search

- Can export file in NIST MSP ASCII format to hard drive
- Any spectrum file in any window in NIST search
- Left click to select entry, then right click and select Export Selected
- Can edit the MSP file with Notepad if you want
- Import in SearchIt for processing using “File/Open Spectrum or Structure”
- Very well demonstrated in video
- Process as normal including library search

The screenshot shows the NIST search interface. At the top, a table lists search results with columns for index, type, and description. Below the table is a bar chart showing the distribution of results across a range of values. At the bottom, a table provides detailed search results with columns for index, library, match count, R.Match, Syn, and DBs.

#	Lib.	Match	R.Match	Syn	DBs
69	M	344	475	7	4
70	M	412	474	1	0
71	R	468	473	4	5
72	R	468	468	36	8

A context menu is open over the table, with 'Export Selected' highlighted. Other menu items include Library Search, Structure Similarity Search, Cut, Copy, Paste, Select All, Send To, Import, Insert Clipboard Structure, Copy Structure to Clipboard, Insert Clipboard Spectra, Copy Selected to Clipboard, Print, Print Preview, and Properties.

The screenshot shows the KnowItAll Informatics System 2023, Analytical Edition menu. The menu is open, and 'Open Spectrum or Structure...' is highlighted. Other menu items include New Search, Close, Close All, Edit Report Templates..., and Exit. The keyboard shortcuts for these items are Ctrl+N, Ctrl+W/F4, and Alt+F4 respectively.

Conclusions

- Very easy to transfer spectra from KnowItAll to NIST for processing
- Easy to “switch to caller” from NIST back to KnowItAll program that sent the spectrum
- Reasonably easy to transfer spectra via NIST MSP text file to KnowItAll SearchIt

NOTE: Be sure to see my other videos for Mass Spec KnowItAll training on my personal website