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.

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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
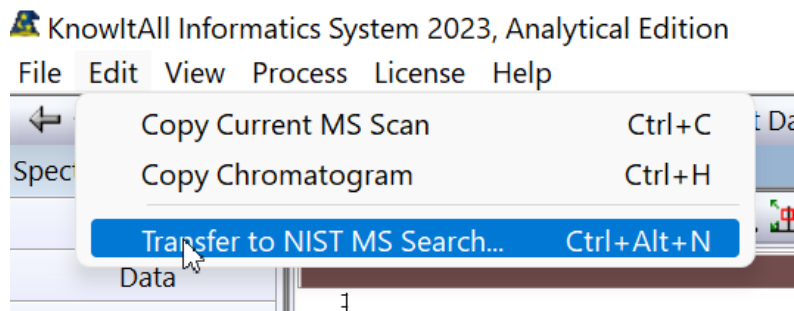
Video Course on Using NIST Search

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
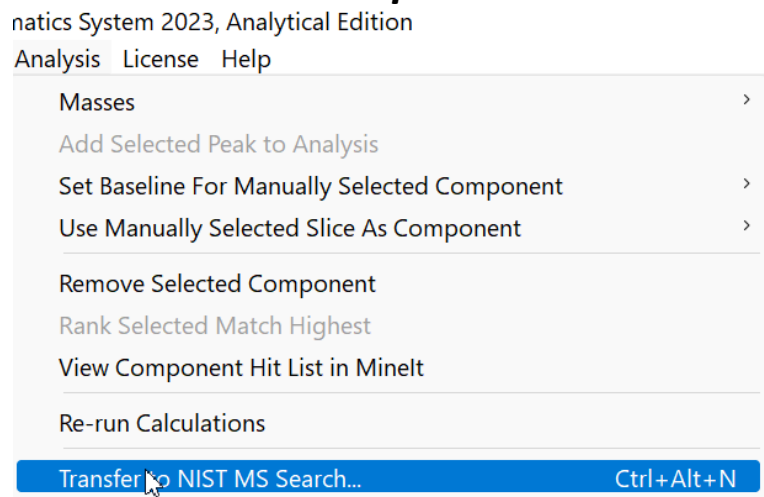
Can Transfer to NIST Easily from KnowItAll in Three Programs

➢ 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
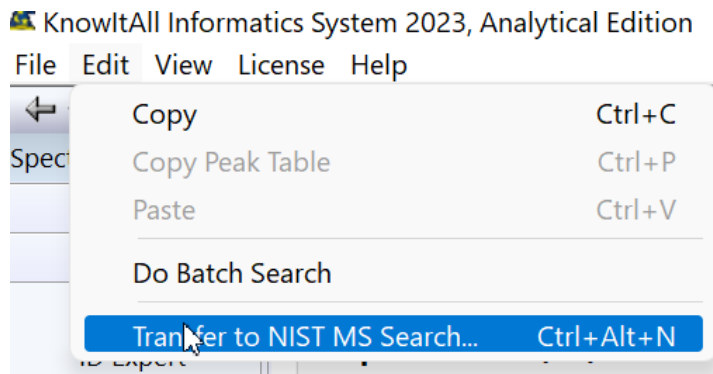➢ Easily return to KnowItAll with "Switch to Caller" arrow in NIST Search
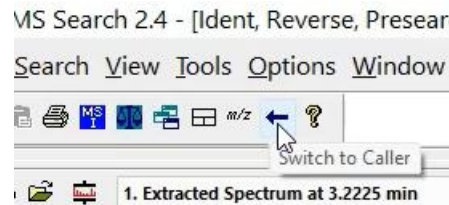
ProcessIt

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

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**