KnowItAll
Mass Spectrometry
Training

Vendor Neutral Data Processing Solution for Spectral Analyses

WILEY

"Making User Library Using PubChem & MS Interpreter"

James Little
Mass Spec Interpretation Services

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

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

Link to Training

Sept 18, 2022

Skills Needed from Previous Videos and Handouts

- ProcessIt for obtaining an EI spectrum from a GC-MS file
- SearchIt/MineIt for searching a mass spectrum
- Tips for drawing structures using ChemWindow

NOTE: Internet links to my FREE course on using NIST MS Interpreter can be found in the associated handout for this video

Another Useful Reference on Databases

Quick Reference Guide

KnowItAll
Analytical Edition

Copyright © 2023 by John Wiley & Sons, Inc. KnowItAll is a trademark of Wiley in certain jurisdictions.

WILEY

Fall 2022

Prepared By
O. David Sparkman

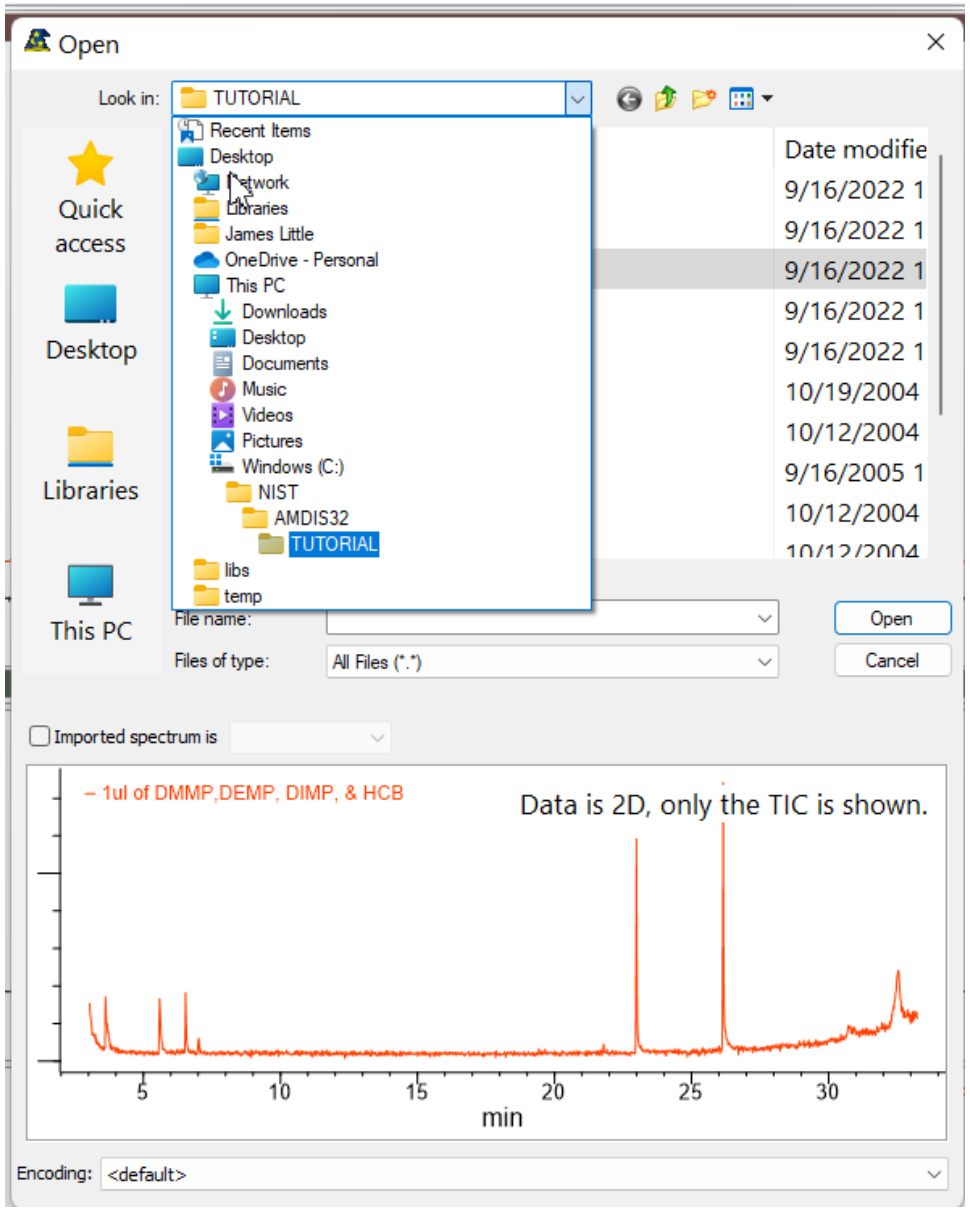
How to Use KnowItAll Mass Spectrometry Applications

NOTE: *Link to Quick Reference* Guide found on my personal website

File Used for Demonstration

File supplied with AMDIS NIST Software in their Tutorial Folder

EAI008.D



Process for Creating User Library (Database)

- Create a user library (database) in MineIt
- Obtain a spectrum for first entry using ProcessIt
- Transfer to MineIt
- Draw a structure in ChemWindow
- Transfer to MineIt and add to first record
- Check quality of spectrum using NIST MS interpreter in MineIT
- Add any fields of interest using PubChem option in MineIt
- Add a comment field
- Continue process to add a second record
- Check by picking one of the entries added and search

Training for NIST MS Interpreter to Understand EI Fragmentation

- The use of MS Interpreter can be found in links shown below
- Will take a little effort on user to become proficient

Links to References (click on them)

-video tutorial
-handout for video tutorial
-other useful references

Other Training of Newly Released Wiley KnowItAll Mass Spec Software on My Website

James Little
Website: "Little Mass Spec and Sailing"
https://littlemsandsailing.com/

Link to Training