

# KnowItAll Mass Spectrometry Training

*Vendor Neutral Data Processing  
Solution for Spectral Analyses*

WILEY



KnowItAll™

## **“Overview of KnowItAll Software for Unknown Identifications in EI GC-MS Analyses”**

James Little  
Mass Spec Interpretation Services

Handouts for Videos:

Website: “Little Mass Spec and Sailing”

<https://littlemsandsailing.wordpress.com>

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

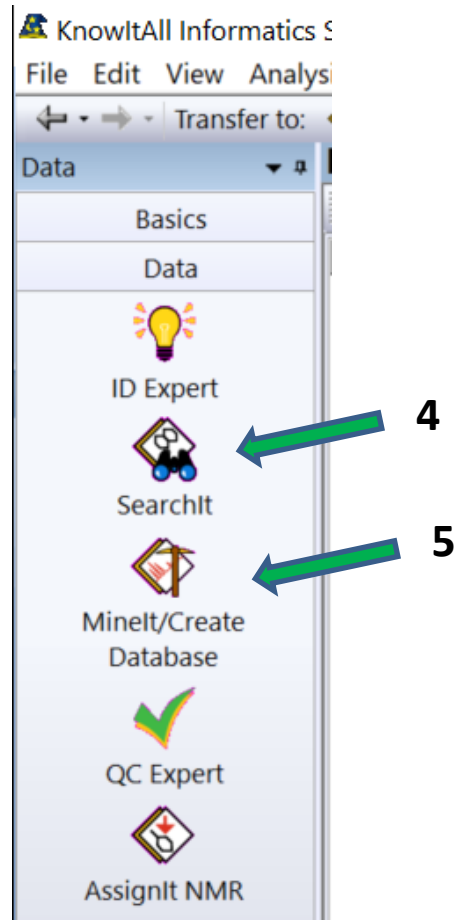
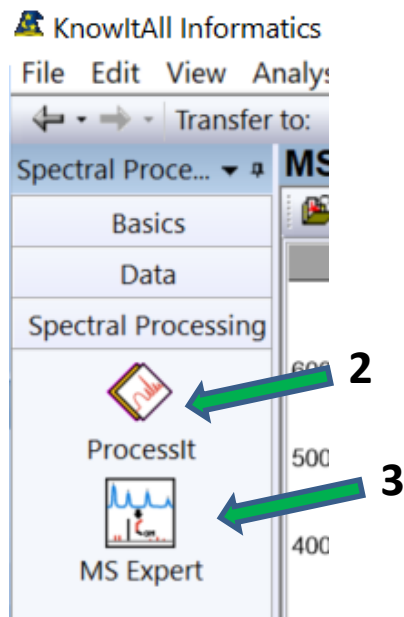
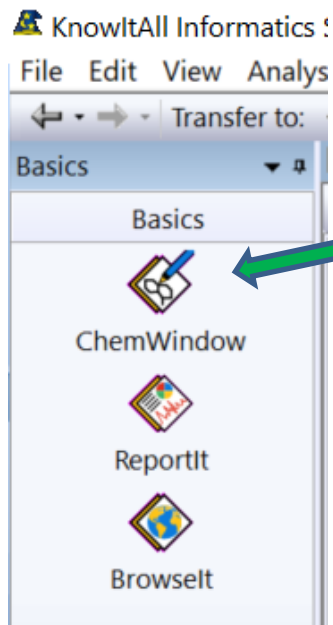
## 5 Primary Software Functions

- ProcessIt:** Manually process nominal and accurate mass EI GC-MS files
- SearchIt:** Manually search EI spectra, structures, names, etc.
- Minelt:** Display EI manual search results
- MS Expert:** Automatic deconvolution of nominal and accurate mass EI GC-MS files
- ChemWindow:** Structure drawing program

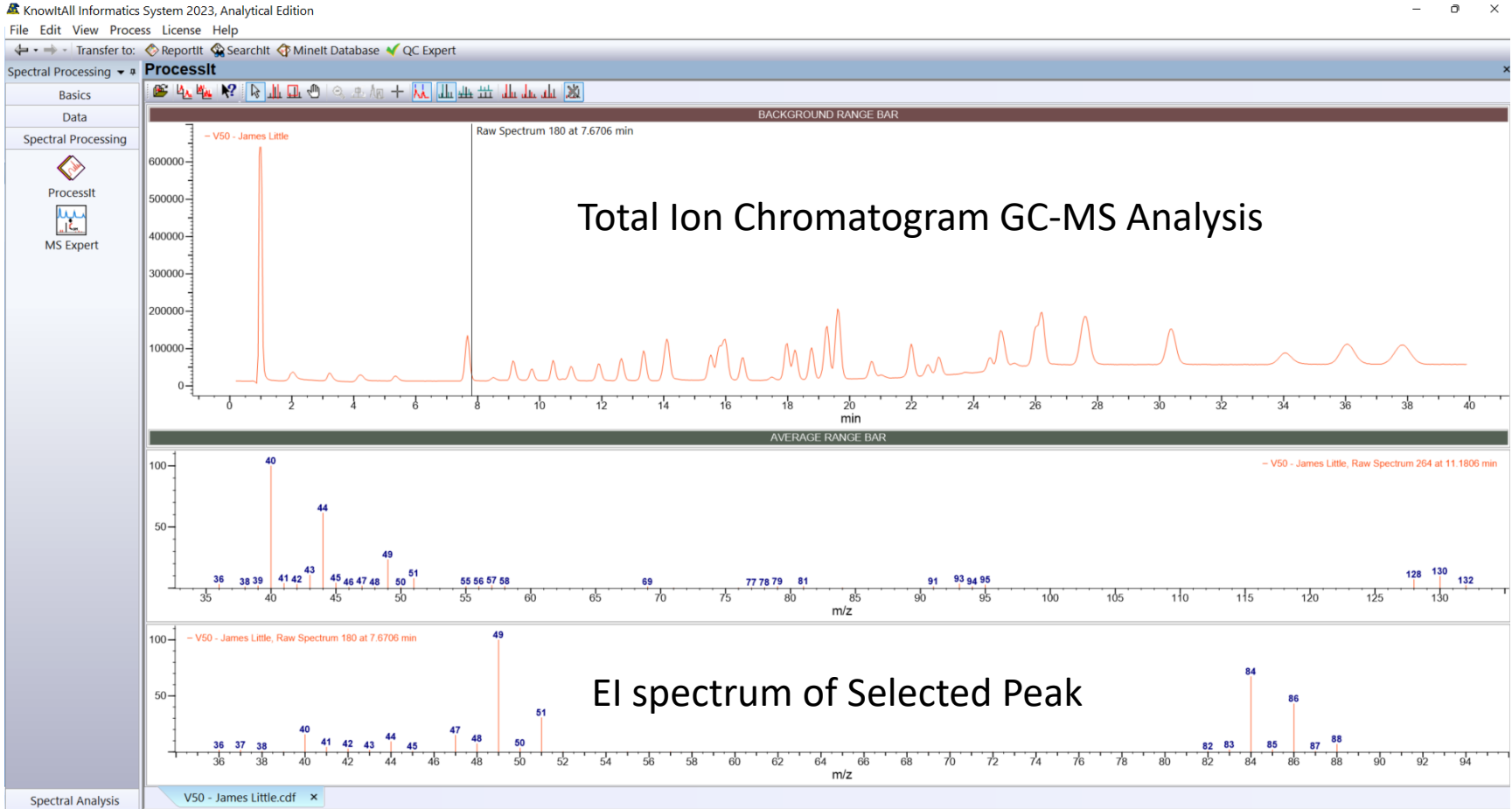
➤ **Also**, the new novel Adaptive MS search greatly extends the identification capabilities for compounds **not** present in EI libraries!

➤ Discussed in detail in another video

# Left Side Bar for Selecting 5 Functions

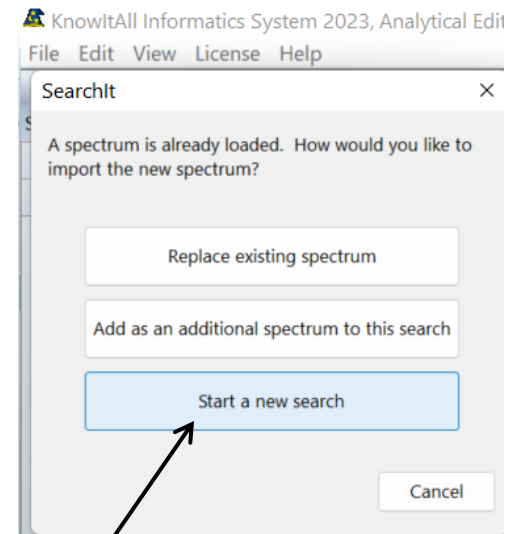
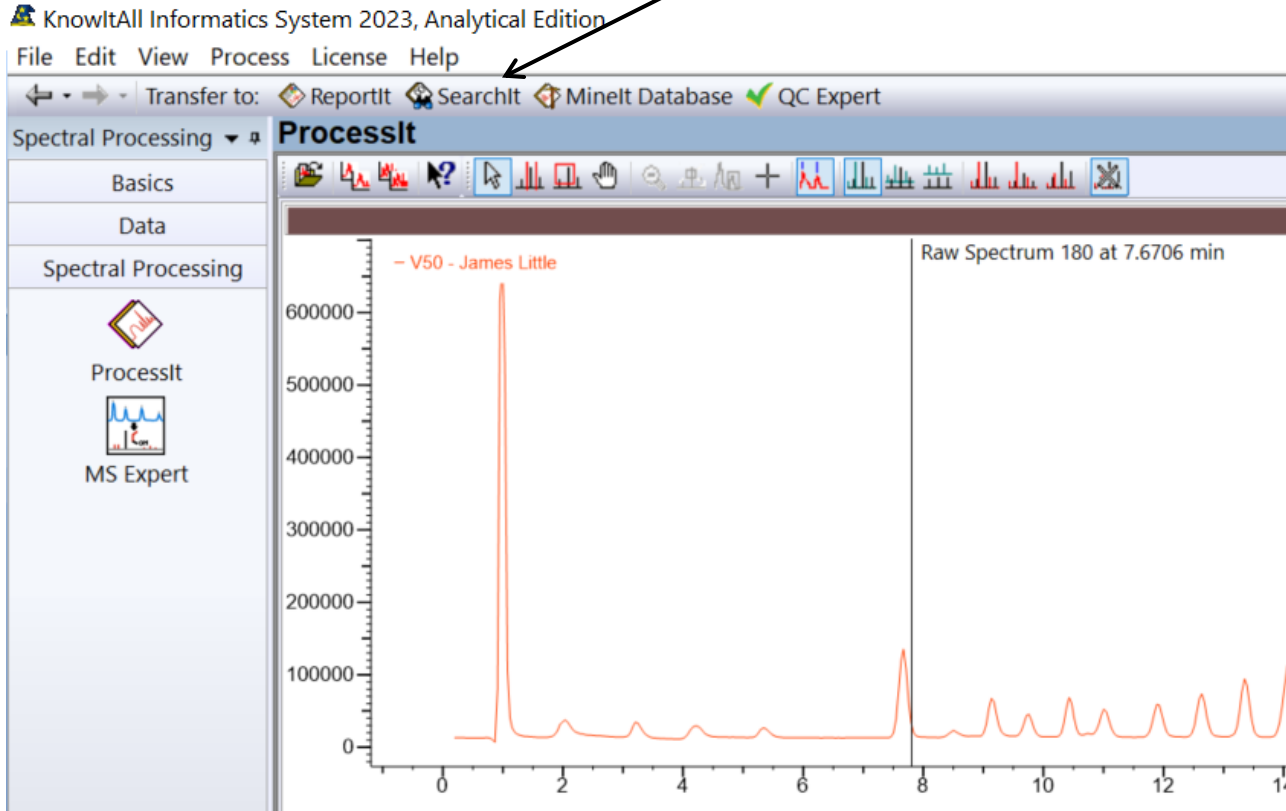


# ProcessIt for Manually Processing EI GC-MS Data



# Sending Selected EI Spectrum to SearchIt Window

Left click on SearchIt



Left click on "Start a new search"

# SearchIt Window to Define Search Parameters Such as Libraries, Types of Search, etc.

KnowItAll Informatics System 2023, Analytical Edition

File Edit View License Help

Transfer to: ReportIt ID Expert Minelt Database QC Expert ProcessIt

Spectral Processing ▾ **SearchIt**

Search Profiles: <no profile>

Number of components: 1 (Single) Search Method: Dot-Product (Cosine)  Adaptive Search Molecular m/z:  Reverse Search

**Spectrum MS (GC)**

Spectrum

Peaks

Structure

Property/Name

**Search Databases**

**User-Select**

All Compounds

Pure Compounds

Hit List Size Limit: 50  All Hits

Set Parameters then "Search"

# Search Results Shown in Minelt >1.2 Million Spectra Searched

KnowItAll Informatics System 2023, Analytical Edition

File Edit View Database Hit List MS Tools Window License Help

Transfer to: ChemWindow ReportIt ID Expert SearchIt QC Expert ProcessIt Analyzelt PredictIt NMR

Spectral Processing ▾ **Minelt**

Basics

Data

ID Expert

SearchIt

Minelt/Create Database

QC Expert

AssignIt NMR

Display Profiles: <no profile>

Lookup Compound: PubChem

Structure/Properties ▾

Structure/Properties

Preferred Properties

Substructs

Sel. Substructs Original Data Files

All Properties Attachments

Name	Value
Name	1,2-Dichlorethane
Alternate Name(s)	Ethane, 1,2-dichloro-
CAS Registry Number	107-06-2
Classification	Pesticides: Insecticides
Exact Mass	97.96901 u
Formula	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>
InChI	InChI=1S/C2H4Cl2/c3-1-2-4/h1-2H2
InChIKey	WSLDOOZREJYCGB-UHFFFAOYSA-N
Molecular Weight	98.959 g/mol
Nominal Mass	98 u
Number of Peaks	41
RI1	682

Add... Edit... Delete

MS (GC)

Table Plot Related Compounds View

HQI	R.HQI	Tag	DE	ID	Name	Spectrum
1	62.74	69.35		MP3 342	1,2-Dichlorethane	
2	55.53	56.28		MSR: 6092	1-Propanol, 2,3-dichloro-	
3	45.90	52.97		MS3 134294	DL-S-methylmethioniniumchloride	
4	44.51	51.53		MS3 710	Methyltetraborane	

Hit selected

Unknown spectrum

Hit selected spectrum

# MS Expert for Automatic Deconvolution and Library Searching of Complex Mixtures in GC-MS

- Chemical background removed
- Coeluting species resolved
- Both nominal and accurate EI GC-MS data
- 50 components characterized in ~6 secs

KnowItAll Informatics System 2023, Analytical Edition

File Edit View Analysis License Help

Transfer to: ReportIt SearchIt Minelt Database QC Expert AssignIt NMR ProcessIt AnalyzIt

Spectral Processing ▾ **MS Expert**

Analysis Profiles: <no profile>

Basics  
Data  
Spectral Processing  
ProcessIt  
MS Expert

Components

RT [m...]	#	Match	Score	HQI	R.H...
0.7241	1	Argon	99.22	99.17	99.68
0.9833	1	Carbamic acid, monoammonium salt	99.95	99.95	99.95
2.0297	1	Methane, chloro-	98.75	98.62	99.92
3.1198	1	Methane, oxybis-	97.68	97.68	97.68
3.2225	1	Methyl bromide	99.61	99.61	99.61
4.2028	1	Ethene, chloro-	97.51	97.51	97.54
5.3466	1	Ethyl chloride	99.82	99.82	99.82
7.6648	1	Methylene chloride	99.79	99.79	99.80
8.5025	1	Acetone	95.43	95.23	97.25
9.1442	1	Dithioxomethane	98.82	98.82	98.82
9.7463	1	Trichloromonofluoromethane	99.85	99.85	99.87
10.4328	1	Ethene, 1,1-dichloro-	99.27	99.26	99.30
10.7473	1	METHANE, DIMETHOXY-	96.45	96.39	97.03
11.0188	1	Methane, bromochloro-	99.38	99.38	99.39
11.9073	1	Ethane, 1,1-dichloro-	98.99	98.99	99.00
12.6332	1	Ethylene, 1,2-dichloro-, (E)-	99.64	99.63	99.69
13.3568	1	METHANE, TRICHLORO-	99.53	99.52	99.53
14.0243	1	1,2-Dichloroethane-d4	93.36	93.36	93.39

Deconvolution

Reference Ion(s): 78 - 83

Parameters:

Contributing Ions: 78  
Energy: 0.0054  
Base Peak Vertex: 55755.5

Resolution:  Automatic

Sensitivity: Low Medium High

Peak Shape Requirements: Low Medium High

Raw Spectrum 458 at 19.2624 min

Match

Spectral Analysis V50 - James Little.cdf



# **More Detailed Training of Newly Released Wiley KnowItAll Mass Spec Software on My Website**

James Little

Website: “Little Mass Spec and Sailing”

<https://littlemsandsailing.wordpress.com>