

# **KnowItAll Software**

---

Training Guide

## Copyright

---

KnowItAll Software Training Guide  
Copyright © 2021 by John Wiley & Sons, Inc.  
All rights reserved.

## Trademarks

---

KnowItAll and ChemWindow are registered trademarks of John Wiley & Sons, Inc. in certain jurisdictions. 3DViewIt, Analyzelt, AssignIt, Browselt, GoodLook, KnowItAll ID Expert, IntelliBucket, KnowItAll AnyWare, Minelt, PredictIt, ProcessIt, QC Expert, ReportIt, Sadtler, SearchIt, SpectraBase and SymApps are trademarks of John Wiley & Sons, Inc.

## Disclaimer

---

John Wiley & Sons, Inc. makes no representations or warranties with respect to the contents of this publication or the accompanying software or databases. John Wiley & Sons, Inc. specifically disclaims any implied warranties of merchantability or fitness for any particular purpose.

John Wiley & Sons, Inc. reserves the right to change or alter this publication and the accompanying software and databases at any time without obligation to notify any persons of such revisions or changes.

No part of this publication or the accompanying software and databases may be reproduced, transmitted, transcribed, stored for electronic or digital retrieval, translated or copied by any mechanical, electronic, magnetic, optical or manual means without expressed prior written consent of John Wiley & Sons, Inc.

## About This Training Guide

This training guide will lead you through a series of exercises in the manner of a training course. Each lesson has a folder of example training files associated with it that can be downloaded here: [www.knowitall.com/training\\_files](http://www.knowitall.com/training_files).

Lesson	Description	Application Featured
<b>1 - General Features</b>	<ul style="list-style-type: none"> <li>Explore the interface</li> <li>Learn to transfer data from one application to another</li> </ul>	KnowItAll "Interface"
<b>2 - Simple Spectral Search/Identification</b>	<ul style="list-style-type: none"> <li>Perform a "first pass" analysis of your spectrum against reference spectra</li> <li>Use patented optimized corrections technology to optimize search results</li> </ul>	KnowItAll ID Expert
<b>3 - Searching - IR and Raman</b>	<ul style="list-style-type: none"> <li>Perform basic, peak, structure, and multi-technique searches</li> <li>Create a search profile</li> <li>Limit search range/exclude search regions</li> <li>Perform a spectral subtraction</li> <li>"All" vs. "Pure Compound" search</li> </ul>	SearchIt
<b>4 - Mixture Analysis - IR and Raman</b>	<ul style="list-style-type: none"> <li>Perform mixture analysis</li> <li>Interpret search results</li> </ul>	SearchIt
<b>5 - Functional Group Analysis</b>	<ul style="list-style-type: none"> <li>Browse the knowledgebase of functional groups</li> <li>Correlate peaks from a structure</li> <li>Perform spectral analysis by functional group – IR, Raman, IR Polymers</li> <li>Create user knowledgebases</li> </ul>	Analyzelt (IR, IR Polymer, Raman)
<b>6 - Searching and Mixture Analysis - MS</b>	<ul style="list-style-type: none"> <li>Forward search</li> <li>Reverse search</li> <li>Mixture analysis</li> <li>Adaptive search (similar compound search)</li> </ul>	SearchIt
<b>7 - Create Databases</b>	<ul style="list-style-type: none"> <li>Create a database with spectra, structures, properties</li> <li>Batch import spectra, structures, properties, PubChem properties</li> <li>Create display profiles</li> </ul>	Minelt/Create Databases
<b>8 - Drawing Structures &amp; Reactions</b>	<ul style="list-style-type: none"> <li>Use basic ChemWindow tools to create and edit a structure</li> <li>Create chemical reactions</li> </ul>	ChemWindow, ReportIt
<b>9 - Creating Reports</b>	<ul style="list-style-type: none"> <li>Use pre-defined report template</li> <li>Create customized templates</li> </ul>	ReportIt
<b>10 - Data Mining &amp; Analysis</b>	<ul style="list-style-type: none"> <li>Use patented Overlap Density Heatmaps for visual data mining</li> </ul>	Minelt

	<ul style="list-style-type: none"><li>• Create an overlap consensus spectrum</li></ul>	
<b>11 - Quality Control Analysis</b>	<ul style="list-style-type: none"><li>• Set up an administrator account</li><li>• Select a standard and compare samples</li></ul>	QC Expert