

What's New in KnowItAll 2021



KnowItAll is better than ever with more tools for analysis, new databases, improved integration with Microsoft Office and accessibility features. We've also expanded KnowItAll's industry leading IR and Raman capabilities with feature updates for more intelligent mass spectral interpretation.

Below is a detailed summary of exciting updates in the 2021 release for our customers and partners. Access to features and data depends on the user's license (edition, etc.)

Software Features & Updates

General Features

- Thorough quality reviews to ensure feature stability and improve user experience
- Enhanced accessibility features, including keyboard access to menus, icon audio narration, tool tips

Advances for MS in this Release

- **NEW! Adaptive Search technology for MS (Patent Pending)** - When matching an unknown spectrum against a reference, this technology finds matches similar to the unknown but have additional or missing selective fragment(s). It then suggests what might be causing the differences, where possible. This feature provides tremendous insights into structural possibilities to explore when there is not an exact match and, ultimately, can lead to more intelligent identification.
- **NEW! MS Mixture Analysis** – This powerful feature, already available for IR and Raman, is now available for MS in this release. In the KnowItAll SearchIt application, you can perform a multi-component search by selecting the number of components to search. The result is a series of composite spectra, accompanied by the individual component spectra that comprise the composite and a residual spectrum (difference between the query spectrum and the composite spectrum).
- **NEW! Reverse Search** – This search finds matches for peaks in the reference spectrum and ignores peaks which are only found in the unknown spectrum.
- **New MS search algorithms and additional MS file formats supported** -Includes NIST *.smp (single or multiple spectra) and high-res LC-MS (mzML, mzXML, MGF, MSn, Mz5)

Additional Updates by KnowItAll Application

SearchIt™

- Exact Mass Search now allows the user to include +/- adducts (i.e. H+, H-, Na+)
- Fast Property Search: new quick look up for the most common properties
- View unknown and reference peak tables in results
- New views to compare spectra: Butterfly (places unknown query spectrum on the positive Y-axis and reference on the negative Y-axis) and Subtraction (allows you to view the difference spectrum)

Minelt™

- Addition of property calculators for single or batch calculations (elemental, isotopic, C-13 NMR prediction, bad baseline indicator, baseline analysis: area difference, SPLASH ID), various masses (average, exact, nominal)
- A R.HQI (Reverse Hit Quality Index) column appears in results list when the user performs a reverse search of a mass spectrum
- Users can send a spectrum-structure pair from a user-created KnowItAll database to NIST MS Interpreter or integrate the NIST Retention Time Calculator (Copy calculator to "C:\Program Files\KnowItAll\Bin" folder)
- **The DEA Controlled Substance Regulation Predictor** rule base was updated and expanded. It can be used to classify chemical structures in KnowItAll user databases (via Minelt application – batch property prediction). (version 2021.1 in ChemWindow and Spectroscopy editions)

ChemWindow®

- Improved Windows Object Linking & Embedding (OLE) features for in-place editing and integration with Microsoft Office
- OPSIN Name2Structure for name to structure conversion (option added to "Chemistry" menu)
- Elemental and isotopic calculators now available (under the "MS Tools" menu)
- Reintroduced reaction drawing and reaction file support: supports RInChI chemical identifiers reactions and CDX/CDXM files

Installation / OS Updates

- Due to increased computational power, KnowItAll 2021 does not support the Windows 32-bit operating system (OS). The supported OS is Windows 10 64-bit. Customers that require a 32-bit version of KnowItAll can still download a 32-bit version of KnowItAll 2020 at www.knowitall.com/download.
- If you download KnowItAll from www.knowitall.com/download, you will notice a change in the install process; KnowItAll will now prompt you to select and then download the databases. NOTE: When installing from a USB the installation remains the same: KnowItAll will install the IR & Raman collections by default; during the installation you must choose which additional databases you wish to install.

KnowItAll Edition Updates

- **NEW! Microplastic Classifications Database** is now included with the Spectroscopy Edition as a fast and cost-effective way to classify microplastics of IR / ATR-IR spectra. For identification of microplastic samples, we recommend users subscribe to the comprehensive KnowItAll IR Spectral Library. (version 2021.1)
- Removed Infometrix Engine and Analyzelt MVP application from all editions.
- The ChemWindow Edition will not have spectral search capability and the ATR solvent (WL) database will not be included. For spectral database searching, users should select the KnowItAll Spectroscopy Edition.

Spectral Database Updates

IR Databases

KnowItAll IR Spectral Library - We have added the following new libraries to this collection:

- IR- Sigma-Aldrich Library of Vapor Phase FT-IR Spectra [WSAVX] - 5,245 spectra
- IR - Sigma-Aldrich Library of Flavors & Fragrances FT-IR Spectra [WSAFX] – 2,488 spectra

NMR Databases

We have made changes to our KnowItAll product portfolio for NMR:

- **NEW!** Sigma-Aldrich NMR Library (Annual Subscription) – Access over 26,000 organic compounds.
 - Includes the following databases: Sigma-Aldrich Library of ¹³C NMR Spectra (13,265 spectra) and Sigma-Aldrich Library of ¹H NMR Spectra (13,164 spectra)
 - This is a separate annual subscription
- **NEW!** AIST NMR Library (Annual Subscription) -
 - Access over 25,000 spectra that includes ¹H and ¹³C data (*NOTE: This database will no longer be included in the KnowItAll NMR Spectral Library. It is a separate annual subscription*)

Here's a current summary of KnowItAll NMR database products available:

Product Code	Name	# Spectra
978EALDB04409	KnowItAll NMR Spectral Library (Annual Subscription) Subscription includes: <ul style="list-style-type: none">• Over 894,000 spectra (CNMR, HNMR, XNMR)• KnowItAll ID Expert for one-click basic spectral search	894K+
978EALDB04393	KnowItAll NMR Identification & Prediction Pro (Annual Subscription) Bundle includes subscription to <ul style="list-style-type: none">• KnowItAll NMR Spectral Library• KnowItAll Spectroscopy Edition Software for advanced analyses/prediction	894K+
978EALDB04379	AIST NMR Library (Annual Subscription) Subscription includes: <ul style="list-style-type: none">• Access to over 25,000 spectra (CNMR, HNMR)• KnowItAll ID Expert for one-click basic spectral search	25K+
978EALDB04355	Sigma Aldrich NMR Library (Annual Subscription) Subscription includes: <ul style="list-style-type: none">• Access to over 26,000 spectra (CNMR, HNMR)• KnowItAll ID Expert for one-click basic spectral search	26K+

NOTE: KnowItAll NMR Spectral Library Product Codes: 978EALDB03273, 978EALDB03266 are no longer available.

MS Databases

We have made some changes to our KnowItAll MS subscription product offerings:

- The KnowItAll Wiley Mass Spectral Library offers access to over 870,000 mass spectra from 14 databases including the Wiley Registry

The following libraries are now offered as options:

- The NIST library is now offered separately as a bundle with the KnowItAll Mass Spectral Library subscription
 - Wiley Mass Spectra of Designer Drugs is now offered as a separate subscription option
- SPLASH IDs were added to the Wiley Registry of Mass Spectral Data 12th Edition databases in the collection

Here's a current summary of KnowItAll MS database products available:

Product Code	Name	# Spectra
978EALDB04256	KnowItAll Wiley Mass Spectral Library (Annual Subscription) Includes KnowItAll ID Expert for one-click basic spectral search	870K+
978EALDB04270	KnowItAll Wiley MS Identification Pro (Annual Subscription) Bundle includes subscription to <ul style="list-style-type: none">KnowItAll Wiley Mass Spectral LibraryKnowItAll Spectroscopy Edition Software for advanced analyses	870K+
978EALDB03242	KnowItAll Wiley Mass Spectral Library + NIST (Annual Subscription) Bundle includes: <ul style="list-style-type: none">Subscription to KnowItAll Wiley Mass Spectral Library + NIST (EI data)Also includes USB with perpetual license to NIST Library/Software (ISBN: 9781119750291)*	1.2M+
978EALDB04294	KnowItAll Wiley MS Identification Pro + NIST (Annual Subscription) Bundle includes: <ul style="list-style-type: none">Subscription to KnowItAll Wiley Mass Spectral Library + NIST (EI data) + KnowItAll Spectroscopy Edition SoftwareAlso includes USB with perpetual license to NIST Library/Software (ISBN: 9781119750291)*	1.2M+
978EALDB04331	Wiley Mass Spectra of Designer Drugs GC-MS Library (Annual Subscription) Includes KnowItAll ID Expert for one-click basic spectral search	31K+

*Per license must be used on the same computer as KnowItAll subscription.

AntiBase - The Natural Compound Identifier Database

- Properties were mapped to and replaced with KnowItAll properties for better data mining