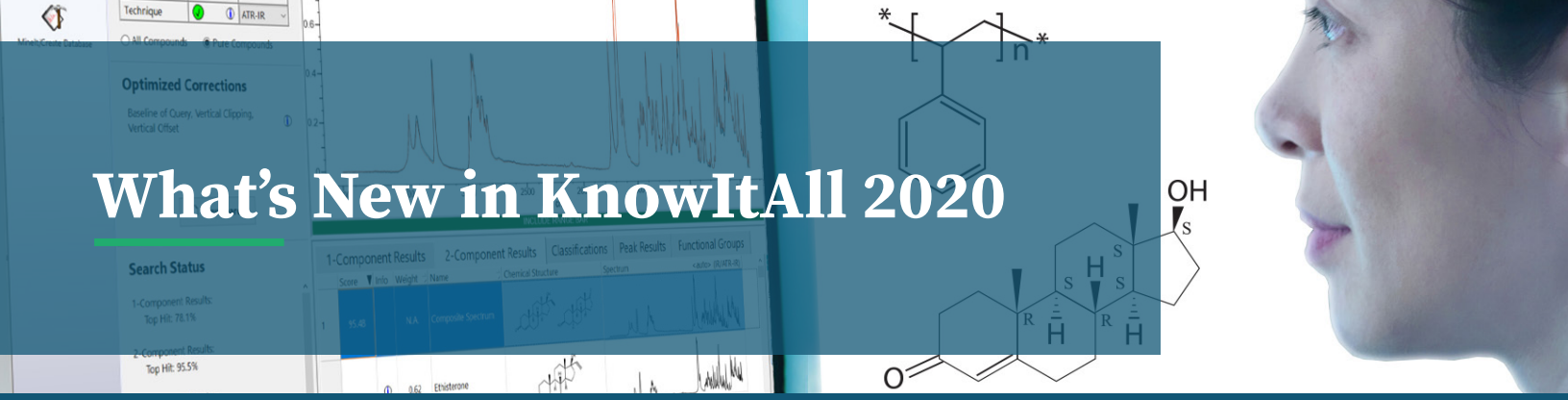

What's New in KnowItAll 2020

Wiley Science Solutions

This document highlights new features in Wiley's KnowItAll 2020 software and databases. Access to features depends on your KnowItAll license. Spectral library access requires a subscription.

KnowItAll Spectral Library Subscriptions

Added over 42,800 spectra—bringing the collection to over 2.4 million spectra—**the world's largest**.

- **KnowItAll Mass Spectral Library** – Added over 42,800 spectra. Now with access to over 1,210,000 spectra
  - The 12th Edition MS databases now include chemical classifications and calculated Kovats retention indices
  - The 12th Edition MS databases replace the 11th Edition MS databases
  - **NEW!** MS - Wiley Registry of Mass Spectral Data 12th Edition – **725,560** spectra
  - **NEW!** MS - Wiley Registry of Mass Spectral Data 12th Edition Legacy Spectra – **2,082** spectra
  - **NEW!** MS - Wiley Registry of Mass Spectral Data 12th Edition Excess Replicate Spectra – **27,742**
  - **NEW!** MS - Wiley Registry of Mass Spectral Data 12th Edition Low-Quality Spectra – **61,906** spectra
  - **NEW!** MS - Wiley Mass Spectra of Designer Drugs 2020 – **29,371** spectra
    (replaces the Wiley Mass Spectra of Designer Drugs 2019)

Wiley also offers the following

- **KnowItAll IR Spectral Library** – Access over 264,000 spectra
  (The Merck and Canadian Forensic IR databases are no longer part of the collection , nor can they be purchased as standalone products)
- **KnowItAll Raman Spectral Library** – Access over 25,000 spectra
- **KnowItAll NMR Spectral Library** – Access over 920,000 spectra
- **KnowItAll UV-Vis Spectral Library** – Access over 30,000 spectra

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KnowItAll Software Updates

Below are new features by application within the KnowItAll software.

KnowItAll ID Expert

- **Now with Integrated Deformulation Capability** - To streamline user workflow for spectral identification, the KnowItAll deformulation functionality has been integrated into ID Expert (formerly Deformulation Expert was a separate application). Users can choose to search all licensed databases (including commercial compounds) or all licensed pure compounds.

- **Classify IR Spectra for Designer Drugs** - Send your unknown spectrum for quick classification using our new IR Designer Drug Models. Compound classes include: Amphetamines, Anabolic Steroids, Barbiturates, Benzodiazepines, Cannabinoids, Cathinones, Cocaine-Type Substances, Opioids, Phencyclidine-Type Substances, Phenethylamines, Piperazines, Steroids, Tryptamines. This new feature might be used, for example, to screen IR spectra for drug-like properties in order to flag for further testing.

SearchIt

- **Simplified Interface** – The new interface clearly defines the parameters the user may choose for their search on a single screen in a much more intuitive and logical way. Like ID Expert, the user can also choose to search all licensed data intelligently linked by not only structure but Name, CAS Registry Number, InChI, InChIKey or synonyms or select specific databases using the "User-Select" option.

- **Integrated Mixture Analysis** – To streamline user workflow for spectral search, the KnowItAll mixture analysis functionality has been integrated into SearchIt (formerly Mixture Analysis was a separate application). From the interface, the user can also include and/or exclude specific known components.

- **Enhanced Simultaneous Multi-Technique Search** – KnowItAll has improved its ability to search unknown spectra from multiple techniques simultaneously and visualize the results on a scatter plot. In this release the "All Compound" search intelligently links records from the various techniques by structure, InChI, InChIKey, CAS Registry Number, Name, Synonym to increase the chances for cross-technique identification.

- **Correlation Algorithm has been updated.**

MineIt

- **Increased Chemical Intelligence with NEW Related Compounds View** – Increase insight into your analyses by further exploring a fuller view of compounds related to your results. This view interconnects all available reference data by structure, name, synonym, and CAS registry number to add an exceptional level of chemical intelligence to the entire platform and further expand knowledge about the results.

- **DEA Controlled Substance Prediction** – Now you can predict the Drug Enforcement Agency classification of chemical structures drawn in a KnowItAll user database. Perform a batch property calculation for your database using this integrated rule-based prediction system.

ProcessIt

- All processing features have been combined into a single application. Instead of opening a separate application for each technique, KnowItAll detects the type of spectrum opened and presents the processing options possible for that technique.

AnalyzeIt

- The AnalyzeIt IR, Raman, and IR Polymer applications have been combined into a single application to further simply the KnowItAll interface and workflow.

ChemWindow

- Users will immediately notice a dramatic improvement to the interface and tools that make it easier to move, highlight, and select objects.
- Added a new comprehensive set of pre-defined substituent fragments.
- Sophisticated “fuzzy” structure representation features have been expanded, including “and,” “or,” and “not” Boolean logic relationships among fragments.

Additional Updates

- **New file formats** – added for Metrohm and Hellma.
- **New KnowItAll Spectroscopy Edition** – This new KnowItAll package offers solutions for IR, MS, NIR, NMR, Raman, UV-Vis, & Chromatography.
- **Retired Editions** - The KnowItAll Analytical and Vibrational Spectroscopy editions are retired with this release.