From the Leader in Spectral Data

KnowItAll Solutions for MS

Powerful Software. Quality Data. Results You Can Rely On.

KnowItAll offers solutions to identify, analyze, and manage your MS data. Combined with the world's largest spectral reference databases, it provides one of the most advanced technologies available for fast, reliable spectral analysis.

With the NEW KnowItAll 2023, Wiley continues to expand KnowItAll's MS capabilities, with tools to automate mass spectrometry processing and accelerate analysis workflows.

By combining all the tools and data you need for effective MS analysis into a single, easy-to-use interface, KnowItAll will **save you time, improve workflow, and increase your ability to reach conclusions** from your data.

Key Features

Automated Non-Targeted GC-MS Analysis
Spectral Search / Processing
Database Building / Management
Integrated Toolsets for Structure Drawing, Reporting, & More
Comprehensive High-Quality Libraries of MS Reference Spectra*
Supports Multiple Vendor/Technique (MS, NMR, IR, Raman, UV-Vis) File Formats

*Subscription required to KnowItAll Spectral Libraries.

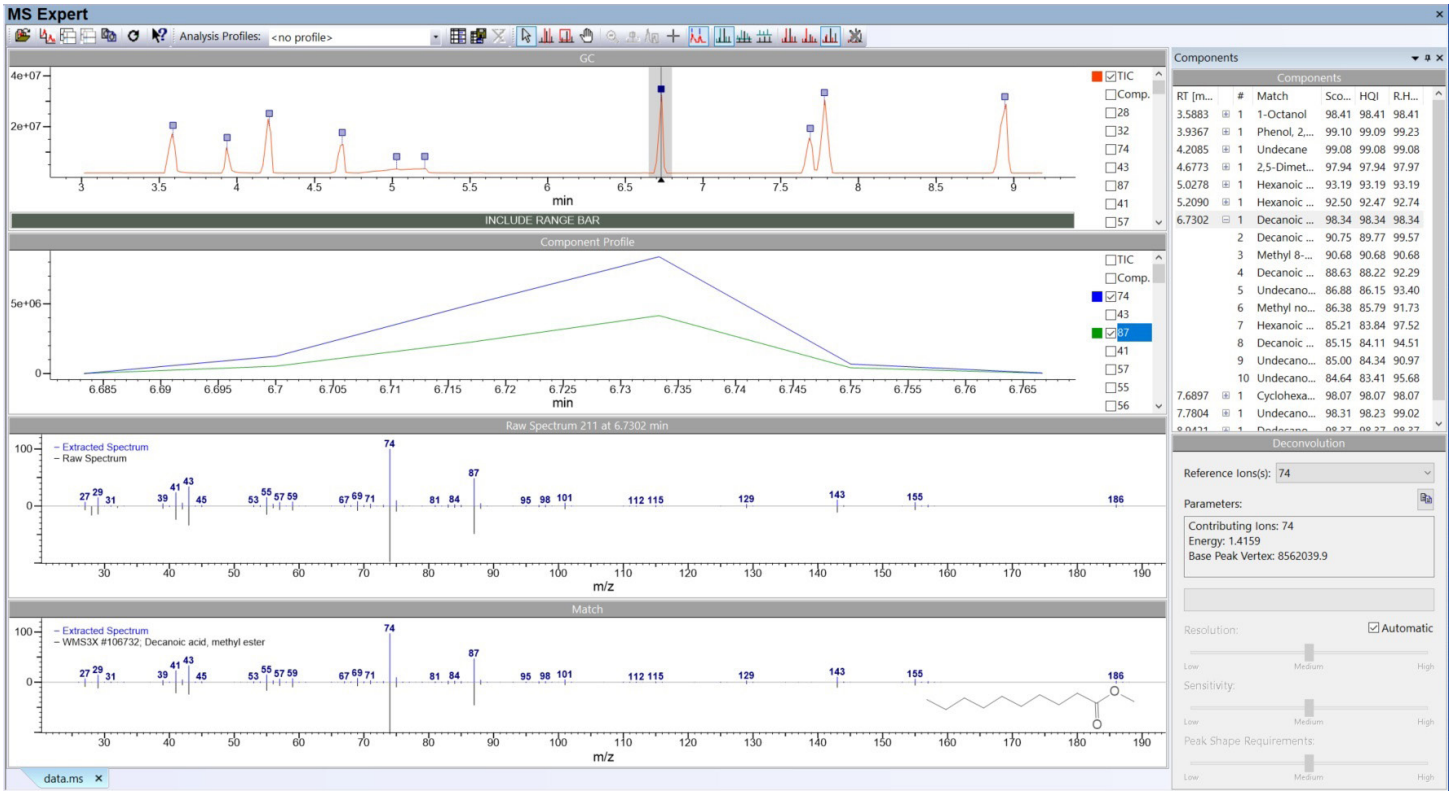
WILEY

Automated Non-Targeted GC-MS Analysis

NEW! MS Expert - Combines Deconvolution with Spectral Search into an Automated Workflow

GC-MS data analysis can be time consuming, especially when examining complex analytes. The new MS Expert automatically processes, deconvolutes, and analyzes GC-MS data.

Combined with KnowItAll's fast database search, it accurately suggests matches to knowns and allows unknowns to be further examined.



Whether you're an expert or beginner, this new MS technology from Wiley can save you hours of manual analysis time by combining fast, flexible deconvolution with an integrated reference database search into a single, automated workflow to identify components.

How Does It Work?

Simply import a GC-MS data file and the software automatically deconvolutes the TIC into components. All extracted component MS spectra are then automatically searched against reference libraries* to find matches. Results are shown as a hit list for each component.

Unidentified components or components with low match scores can then be sent to KnowItAll's SearchIt tool for manual investigation. In SearchIt, one can use adaptive search to match similar components or use mixture analysis to separate coeluted components.

Key Features

- Automatic GC-MS data deconvolution
- Automatic search of component's extracted MS spectra to match against comprehensive KnowItAll MS spectral references libraries*
- Also allows user databases to be included in the search
- Simultaneous regular spectral search and reverse search
- Adjustable match score calculations based on regular spectral search and reverse search HQI values
- Can analyze unit mass data as well as accurate mass data
- Display presents TIC, component profile, extracted spectrum vs raw spectrum, extracted spectrum vs. matched reference spectrum graphs, as well as the matched reference data structure
- Allows user to manually pick additional peaks from the TIC
- Select TIC regions for analysis
- Adjustable analysis sensitivity parameters
- Adjustable input data resolution set-up for accurate mass data
- Seamlessly transfer components which are not matched well to reference spectra to SearchIt for manual examinations using either Adaptive Search or mixture analysis
- Generate reports with results
- Supports multiple instrument types and vendor formats (www.knowitall.com/formats)
- Optimized for speed and performance

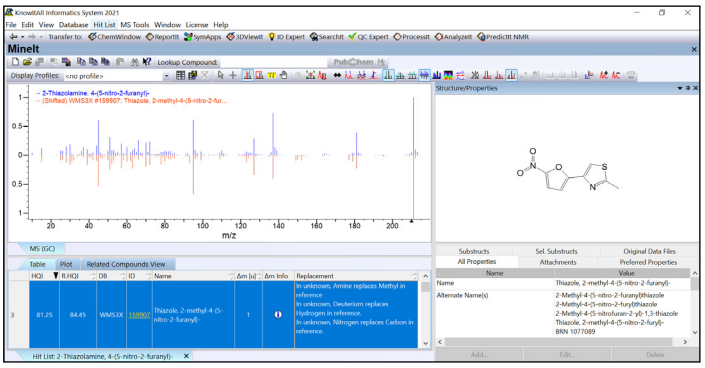
*Subscription required to KnowItAll Spectral Libraries.

Spectral Search

Sophisticated MS Search for Confident Identification & Classification

Wiley offers sophisticated tools to search and compare unknown mass spectra with KnowItAll's high-quality reference spectra* or user generated databases.

With fast search speeds, powerful algorithms, and advanced technologies, Wiley aims to deliver results you can rely on.



Key Features

- Import spectra to search and compare against user-generated databases or KnowItAll libraries
- Searches are fully customizable and driven by powerful algorithms
- Search by name, structure, substructure, properties, spectra, and peak—in any combination
- Perform mixture analysis for multiple components
- MS Adaptive Search (patent pending) for insight into structural possibilities to explore
- MS Reverse Search
- Include or exclude regions from your searches
- Include or exclude known components in mixture analyses to narrow results
- Manually select peaks or use automated peak picking capability
- Perform simultaneous multi-technique search with spectra from other techniques to orthogonally validate for more confident analyses
- Various views: overlay, offset, stack, butterfly, subtraction, etc.
- Supports multiple instrument types and vendor formats (www.knowitall.com/formats)
- Optimized for speed and performance

Tools That Set KnowItAll Apart

NEW! Wiley's Patent-Pending Adaptive Search for MS: This technology finds spectral matches that are 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 insight into structural possibilities to explore when there is no exact match. Ultimately, this may lead to more intelligent and confident identification and confirmation.

Mixture Analysis of MS Spectra: One of the most powerful features is KnowItAll's ability to analyze mixtures. When searching an unknown against a reference database, you can choose to search for multiple components. The result is a series of composite spectra, each accompanied by the individual component spectra that comprise the composite spectrum, as well as the residual spectrum (difference between the query and the composite spectrum). Composite spectra are then ranked by how closely they resemble the query spectrum.

*Subscription required to KnowItAll Spectral Libraries.

Processing

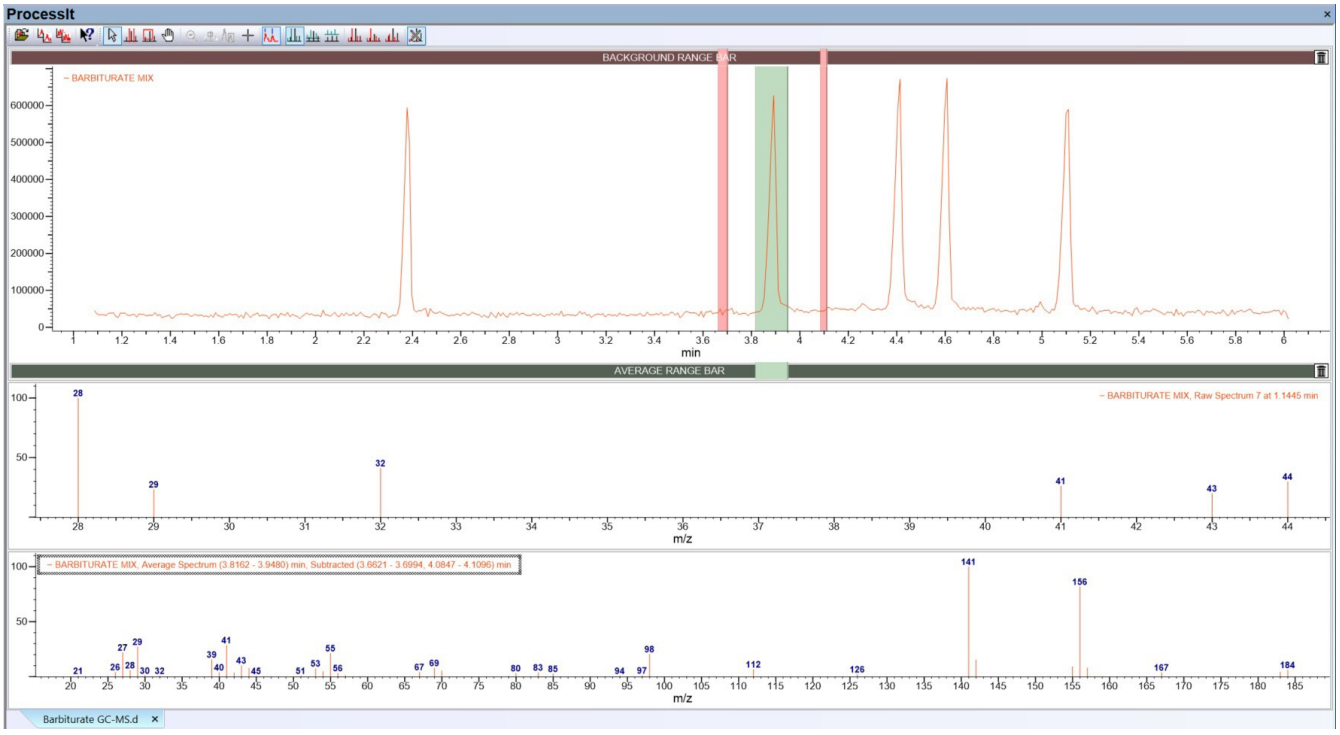
GC-MS Data Processing

With ProcessIt, users can view and select a mass spectrum or the average of mass spectra and define the background. The selected mass spectrum or extracted spectra can be transferred for database searching or imported into a user database.

Selected Ion Chromatograms (SICs) - ProcessIt allows the display of a selected ion chromatogram. Multiple ion chromatograms can be displayed in the top pane.

Spectral Subtraction - This feature allows calculation of the average mass spectrum and also allows the elimination of background noise via manual background subtraction. Single or multiple ranges for either process can be specified.

As shown in the screenshot below, the lower pane holds either selected MS, selected MS – background (*red bar*), average MS (*green bar*), or average MS (*green bar*) - background (*red bar*).



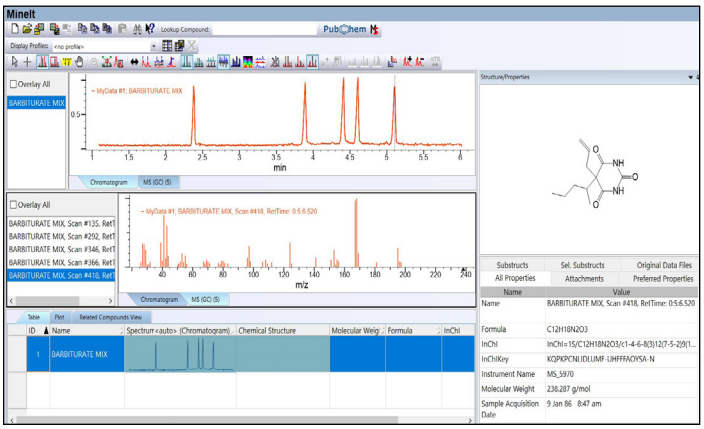
*Subscription required to KnowItAll Spectral Libraries.

Spectral Data Management

Build Single or Multi-Technique Databases from Various Vendors

Because Wiley Science Solution's primary business is spectral databases, KnowItAll is built through years of experience in doing just that—building databases.

Researchers can build searchable databases that include one or more analytical techniques (IR, MS, Near IR, NMR, Raman, UV-Vis), chemical structures, and other meta data. So even if a laboratory's instruments come from multiple manufacturers, KnowItAll can archive the data.

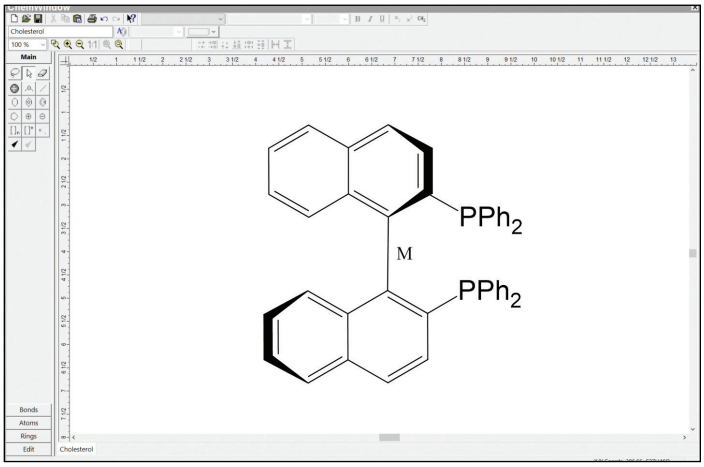


Key Features

- Build databases with MS data or more analytical techniques
- Build databases with multiple spectra in the same record
- One-click import of common instrument file formats or *.csv format (spreadsheet)
- Enhance each record with peak information, structures, and properties, including custom fields
- Import multiple structure formats (with stereo-chemical bonds and identifiers)
- Use "Batch Import and Export" for efficient handling of spectra, structures, and property files
- Supports unrestricted spectral range and resolution - Store spectra at the precise range and resolution at which each spectrum was measured
- Attach spreadsheets, MSDS, and other documents and add hyperlinks to web pages
- Property calculators for single or batch calculations for entire datasets: formula, molecular weight, C-13 NMR prediction, bad baseline indicator, baseline analysis: area difference, SPLASH ID, various masses (average, exact, nominal)
- MS tools to calculate elemental composition and isotope distribution
- Quickly add properties and structures from PubChem to your database
- Categorize structures of controlled substances according to Drug Enforcement Agency regulations
- Fully integrated with other KnowItAll applications for processing, database searching/mining, structure drawing, processing, reporting
- Includes patented Overlap Density Heatmap technology to visualize trends in large datasets

Integrated Tools for Structure Drawing, Reporting, & More

ChemWindow 2D Structure Drawing Program & Communications Tools

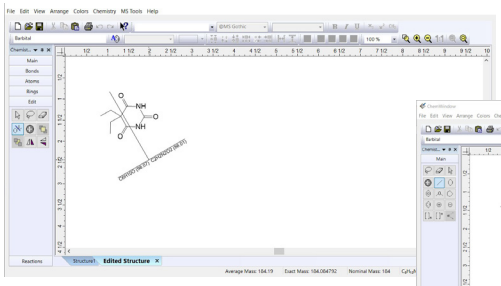


Because structures are critical to your work, we included all the tools you need to streamline your workflow and save time.

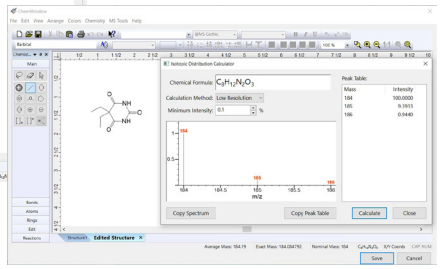
ChemWindow is the software chemists worldwide choose for chemical structure drawing. It provides an advanced set of drawing tools that's easy to use— just click and drag to draw any chemical structure. Access the most comprehensive set of tools to draw rings, bonds, atoms, electrons, charges, chains, arrows, and more.

And with KnowItAll's ReportIt tool, create standard reports, papers, and presentations that include annotations, tables of data, spectra, 2D and 3D structures, and more.

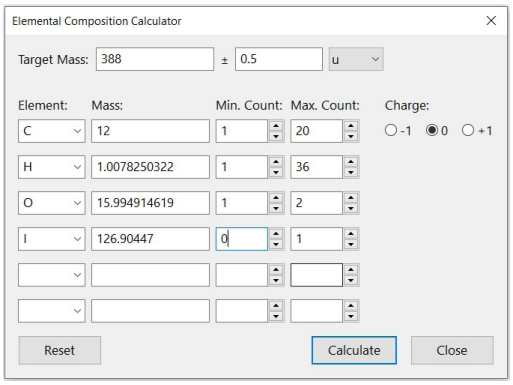
And Many More Value-Added MS Tools!



Mass Fragmentation Tool



Isotopic Distribution Tool

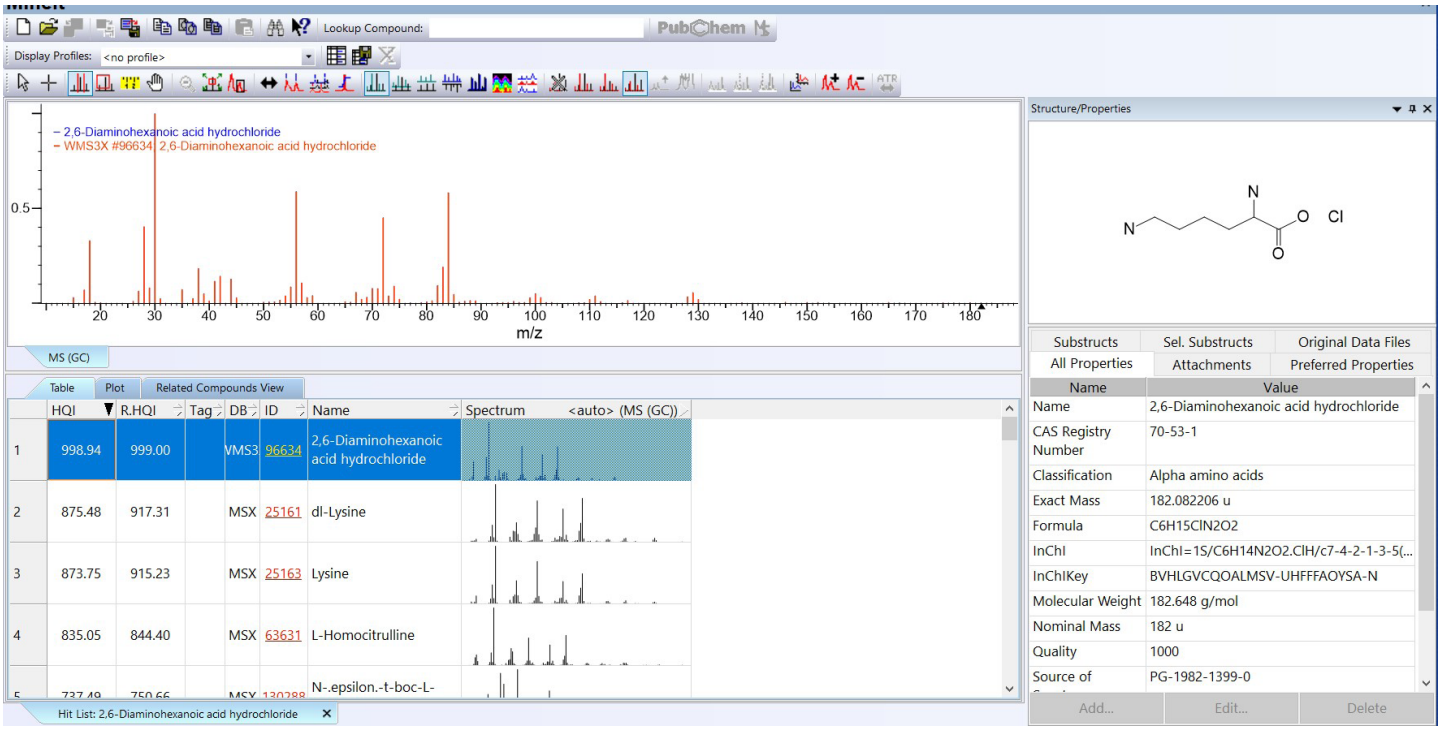


Elemental Composition Calculator

KnowItAll Spectral Libraries

The Most Comprehensive Data for Results You Can Rely On

Spectral Analysis software is not complete without a high-quality database of reference spectra. And with KnowItAll, Wiley offers the best of both!



The **KnowItAll Wiley Mass Spectral Library*** is a trusted data source that provides over 934,000 mass spectra of the highest quality.

- Access 12 MS databases including the renowned Wiley Registry
- Covers a wide range of compounds including organics, drugs, steroids, additives, geochemicals, petrochemicals, biomarkers, industrial compounds, and more
- Along with spectra, records contain physical properties and structures when available
- Includes KnowItAll ID Expert tool for a basic one-click basic spectral search
- Import spectra for identification from most MS instruments
- Access the most recent data as it is added to the library

Increase access to over 1.3 million spectra by adding NIST and other data options.

*Subscription required to KnowItAll Spectral Libraries.

Subscription Options

Product Code	Name	# Spectra
978EALDB04256	**KnowItAll Wiley Mass Spectral Library** (Annual Subscription) Includes KnowItAll ID Expert for one-click basic spectral search	934K+
978EALDB04270	**KnowItAll Wiley MS Identification Pro** (Annual Subscription) Bundle includes subscription to • KnowItAll Wiley Mass Spectral Library • KnowItAll Analytical Edition Software for advanced analyses	934K+
978EALDB03242	**KnowItAll Wiley Mass Spectral Library + NIST** (Annual Subscription) Bundle includes: • Subscription to KnowItAll Wiley Mass Spectral Library + NIST (EI data) • Also includes USB with perpetual license to complete NIST Library & Software (9781119750291)**	1.3M+
978EALDB04294	**KnowItAll Wiley MS Identification Pro + NIST** (Annual Subscription) Bundle includes: • Subscription to KnowItAll Wiley Mass Spectral Library + NIST (EI data) + KnowItAll Analytical Edition Software for advanced analyses • Also includes USB with perpetual license to complete NIST Library & Software (9781119750291)**	1.3M+
978EALDB04331	**Wiley Mass Spectra of Designer Drugs GC/MS Library** (Annual Subscription) Includes KnowItAll ID Expert for one-click basic spectral search	34K+
978EALDB05567	**Food, Flavors, Fragrances, and Related Compounds: GC-MS Library**	13K+

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Compatibility

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Available in English, Japanese, Chinese, French, and German.
Now with accessibility features such as keyboard access to menus, audio narration for icons, tool tips.