

KnowItAll Edition Feature Comparison Chart

● - Included in Edition ○ - Optional

| Component | Description | IR/NIR Edition | Spec Edition | Analytical Edition | Enterprise Edition | Raman Edition | UV-Vis Edition |
|------------------------------------|--|----------------|--------------|--------------------|--------------------|---------------|----------------|
| Data Toolbox | | | | | | | |
| SearchIt™ | Database searching (full spectrum, structure, peak, property, etc.) | ● | ● | ● | ● | ● | ● |
| Minelt™ | Database display and mining | ● | ● | ● | ● | ● | ● |
| Database Building | Build multi-technique† databases with spectra and structures; feature in Minelt | ○ | ● | ● | ○ | ○ | ● |
| Overlap Density Heatmap | Patented technology for visual data mining and analysis | ● | ● | ● | ● | ● | ● |
| CompareIt™ | Data plotting and visualization | ● | ● | ● | ● | | ● |
| AssignIt™ | Add assignments to NMR databases for ¹ H, ¹³ C, and other nuclei | | | ● | ● | | |
| Mixture Analysis | Analyze experimental spectral data of mixtures | ● | ● | ● | ● | ● | ● |
| Batch Property Calculation | Calculate properties for entire databases | ● | ● | ● | ● | ○ | ● |
| Pirouette® Model Support | Use models built in Infometrix Pirouette software | ● | ● | ● | ● | ● | ● |
| Spectral Processing Toolbox | | | | | | | |
| RefineIt™ IR | IR spectrum processing | ● | ● | ● | ● | | |
| RefineIt™ Raman | Raman spectrum processing | | ● | ● | ● | ● | |
| ProcessIt™ NMR | NMR spectrum processing | | | ● | ● | | |
| ProcessIt™ MS | MS and hyphenated MS processing | | ● | ● | ● | | |
| Additional MS File Imports Filters | | | ● | ● | ○ | | |
| Spectral Analysis Toolbox | | | | | | | |
| AnalyzeIt™ IR | IR spectrum/structure correlation | ○ | ○ | ○ | ○ | | |
| AnalyzeIt™ Raman | Raman spectrum/structure correlation | | ○ | ○ | ○ | ○ | |
| AnalyzeIt™ MVP | Multivariate processing for chemometrics and principle component analysis | ○ | ○ | ○ | ○ | ○ | ○ |
| ValidateIt™ | Statistical model validation | ● | ● | ● | ● | ○ | ● |
| AnalyzeIt™ Polymer IR | IR spectrum/structure correlation for polymers | ○ | ○ | ○ | ○ | | |
| Prediction Toolbox | | | | | | | |
| PredictIt™ NMR | NMR chemical shift prediction | | | ● | ● | | |
| Basics Toolbox | | | | | | | |
| DrawIt™ | 2D structure drawing | ● | ● | ● | ● | ● | ● |
| ReportIt™ | Custom reports and publishing tools | ● | ● | ● | ● | ● | ● |
| 3D ViewIt™ | Visualization of 3D structures | | ● | ● | ● | | ● |
| BrowseIt™ | Web portal with useful links for KnowItAll users | ● | ● | ● | ● | ● | ● |
| IUPAC Toolbox | | | | | | | |
| IUPAC DrawIt™ | Convert IUPAC name to structure | ○ | ○ | ○ | ○ | ○ | ○ |
| IUPAC NameIt™ | Convert structure to systematic IUPAC name | ○ | ○ | ○ | ○ | ○ | ○ |
| Other Options | | | | | | | |
| Spectral Databases | Choose from over 100 spectral databases or HavelItAll annual licenses | ○ | ○ | ○ | ○ | ○ | ○ |
| KnowItAll® Enterprise Server | Centralize spectral and chemical information | ○ | ○ | ○ | ○ | ○ | ○ |
| Infometrix Pirouette® Software | Additional chemometrics tools | ○ | ○ | ○ | ○ | ○ | ○ |
| Upgrade Plan | Support and upgrade plan for KnowItAll users | ○ | ○ | ○ | ○ | ○ | ○ |

† Formats supported will depend on the edition of KnowItAll that you choose.

KnowItAll File Formats

KnowItAll helps scientists deal with multiple types of spectral/chemical data and multiple file and instrument formats. Formats supported depend on the edition of KnowItAll licensed. KnowItAll is also capable of importing XY data as well as spreadsheets: Generic X Y data files (*.*) ; text files delimited by comma, tab, etc. (*.csv).

IR

Sadtler IRF files (*.irf)
Bomem files (*.a01)
Bruker files (*.*)
Digilab files (*.dt)
Galactic/GRAMS files (*.spc, *.fir, *.ir, *.rmn)

Generic XY Data files (*.*)
Horiba MDW files (*.mdw)
JASCO files (*.jws, *.j1d)
JCAMP files (*.dx, *.jdx)
JEOL files (*.wsf)

Mattson files (*.ras, *.abs)
PE Spectrum files (*.sp)
Shimadzu IR (*.irs, *.smf)
Spectacle/Shimadzu files (*.irs, *.nmr, *.uvd)
Thermo/Nicolet files (*.spa)

Raman

Sadtler IRF files (*.irf)
Bomem files (*.a01)
Bruker files (*.*)
Digilab files (*.dt)
Galactic/GRAMS files (*.spc, *.fir, *.ir, *.rmn)
Generic XY Data (*.*)

Horiba MDW files (*.mdw)
Horiba NGS files (*.ngsw)
JASCO files (*.jws, *.j1d)
JCAMP files (*.dx, *.jdx)
JEOL files (*.wsf)
JEOL JCAMP files (*.wsf)

Mattson files (*.ras, *.abs)
PE Spectrum files (*.sp)
Renishaw WIREF files (*.wxd)
Shimadzu IR (*.irs, *.smf)
Spectacle/Shimadzu files (*.irs, *.nmr, *.uvd)
Thermo/Nicolet files (*.spa)

NIR

Sadtler IRF files (*.irf)
Bomem files (*.a01)
Bruker files (*.*)
Digilab files (*.dt)
Galactic/GRAMS files (*.spc, *.fir, *.ir, *.rmn)

Generic XY Data files (*.*)
GuidedWave files (*.*)
Horiba MDW files (*.mdw)
JASCO files (*.jws, *.j1d)
JCAMP files (*.dx, *.jdx)

Mattson files (*.ras, *.abs)
PE Spectrum files (*.sp)
Spectacle/Shimadzu files (*.irs, *.nmr, *.uvd)
Thermo/Nicolet files (*.spa)

NMR (processed spectra only)

Bruker Aspect (*.*)
Bruker TopSpin (*.1r, *.fid)
Bruker UXNMR/XWinNMR 1D (1r, fid)
Bruker UXNMR/XWinNMR 2D (2rr)
Bruker WinNMR (*.1r, *.fid)
Galactic/GRAMS files (*.spc, *.fir, *.ir, *.rmn)
Generic XY Data (*.*)

JEOL Alice (*.als)
JEOL Delta NMR files (*.jdf)
JEOL DA-5000 (*.dat)
JEOL GX/GSX/EX-90 NMR files (*.gxd, *.gxp)
JEOL Mario (*.hed)
JCAMP files (*.dx, *.jdx)

MestRe-C (*.mrc)
NUTS files (*.*)
Sparky NMR Files (*.ucsf, *.sf)
Spectacle/Shimadzu files (*.irs, *.nmr, *.uvd)
Varian 1D NMR files (phasefile, data, fid)
Varian 2D NMR files (phasefile)

MS

Agilent / HP ChemStation (*.d; data.ms) Agilent / HP ChemStation (NT) (.msd, *.ms)
ANDI Mass Spec files (*.cdf)
Aneiva AGS-7000 (*.par)
Aneiva AGS-7000 (DOS) (*.par)
Automass (*.spa)
Balzers QuadStar (*.scb)
EPA (*.ep)
Extrel Merlin (*.ms)
Finnigan GCQ (*.ms)
Finnigan Incos (*.mi)
Finnigan Ion Trap (*.dat)
Finnigan ITS-40 (*.ms)
Finnigan Magnum (*.ms)
Finnigan SSX (*.dat)
Galactic/GRAMS files (*.spc, *.fir, *.ir)

Generic XY Data (*.*)
Hitachi (*.mch)
Hitachi M-4100 (ms1.mat)
Hitachi MS Filer (*.msf)
HP RTE Chemstation (*.ms)
JEOL Compliment (*.hed)
JEOL DA-5000 (*.dat)
JEOL DA-6000 (*.dat)
JEOL GCMate (*.lrp)
JEOL JCAMP (*.jsp)
JEOL Mario (*.hed)
JCAMP files (*.dx, *.jdx)
Kratos DS90 (*.rn)
Kratos Mach3 (*.run)
MASPEC (*.mss)
Mass Evolution (*.spe)

Mass Evolution EZScan v4 (*.hrd)
MassLib JCAMP (*.mli)
MatLab (*.mlt)
MSS (*.mss)
MS ChemStation (*.ms)
Nermag SIDAR (*.spe)
Netzsch (*.ntz)
netCDF (*.cdf)
Palisade PAL (*.pal)
PE TurboMass (*.raw;_func, *.dat)
PE QMass-910 (*.mss)
Shrader Systems/Windows (*.lrp)
Shrader System (*.lrp)
Shimadzu PAC200 (*.x)
Shimadzu QP-5000 (*.r)
Spectacle/Shimadzu files (*.irs, *.nmr, *.uvd)

Teknivent Vector/2 (*.tkf)
Teknivent Vector/1 (*.raw)
Teknivent Vector/2 (*.v2s)
Text (*.txt)
ThermoQuest Xcalibur (*.raw)
Varian Saturn (*.ms)
VG 11-250 (*.dat)
VG JCAMP (*.jdx)
VG LabBase (*.hdr)
VG MassLab (*.raw;_func, *.dat)
VG MassLynx (*.raw;_func, *.dat)
VG MassLynx Processed (*.raw;_func, *.dat)
VG ThermoLab (*.lgh)
VG ThermoLab (*.ps)

UV-Vis

Galactic/GRAMS files (*.spc, *.fir, *.ir)
Generic XY Data files (*.*)

JCAMP files (*.dx, *.jdx)
JASCO files (*.jws)

PG Instruments files (*.spd)
Spectacle/Shimadzu files (*.irs, *.nmr, *.uvd)

GC

ANDI Chromatography files (*.cdf)
Galactic/GRAMS files (*.spc, *.fir, *.ir)

Generic XY Data files (*.*)
MS ChemStation files (*.ms)

Spectacle/Shimadzu files (*.irs, *.nmr, *.uvd)

Structure File Formats

ChemDraw files (.cdx)
ChemWindow files (.cwg)
JCAMP files (*.dx, *.jdx)

Hampden files (.hsf)
InChI structure files (*.txt) MDL RXN files (.rxn)

MDL MOL files (.mol)
XYZ structure files (.xyz)

Smiles structure files (*.smi)
DrawIt files (.dsf)

Data File Formats

MDL SDF files (.sdf)

Infomatrix files (*.dat)



Bio-Rad
Laboratories, Inc.