

Spectroscopy



Databases & Software

BIO-RAD

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Databases & Software for Spectroscopy

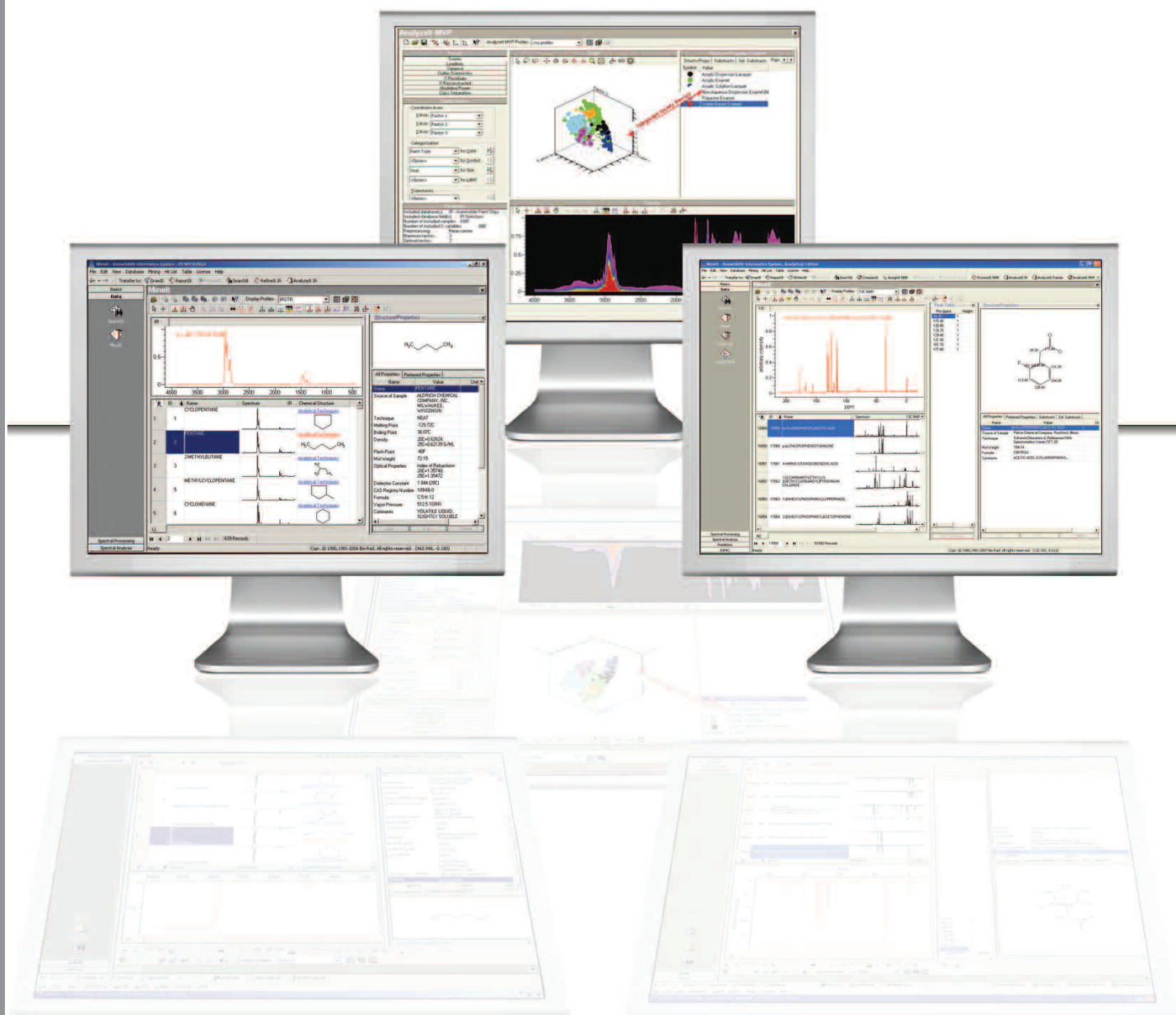
Bio-Rad's Informatics Division specializes in database and software solutions for the scientific community.

Spectral Databases - Over 1.3 Million Spectra, Including Sadtler Data

Bio-Rad is the leading producer and publisher of fully verified spectral databases, with a collection that contains IR, Raman, NIR, NMR, MS, and UV-Vis data covering pure compounds and a broad range of commercial products.


KnowItAll® Software

Bio-Rad specializes in software solutions to manage and analyze *multiple* types of spectral and chemical data in *multiple* file and instrument formats.



Bio-Rad offers over 1.3 million high-quality IR, NMR, MS, UV-Vis, Raman, and NIR spectra (including Sadtler data). Collections cover pure compounds and a broad range of commercial products. They are ideal for interpretation, identification, verification, and classification of spectra. Choose from individual databases or HaveltAll annual licenses.

IR Databases: Polymers & Related Compounds

 Contains Structures

Acrylates & Methacrylates

Product Code 4476

470 Spectra

This database contains spectra of acrylic and methacrylic compounds. It includes a number of polymeric and monomeric compounds that are used in many common products.

Adhesives & Sealants

Product Code 4330

2,070 Spectra

This collection contains a wide range of basic synthetic resins and elastomers, plus cured and uncured commercial end products. Typical products are composed of rubber adhesives, contact adhesives, hot melt adhesives, silicone adhesives, pressure sensitive adhesives, cements, and sealants.

Adhesives & Sealants (Subset A)

Product Code 4230

520 Spectra

The database contains adhesives and sealants in eleven classifications which have been generally established by the adhesives industry. Collection includes basic synthetic resins, elastomers, uncured materials, and cured commercial end products.

ATR of Basic Polymers

Product Code 4485

500 Spectra

Collection of ATR reference spectra of commercially available polymers.

ATR of Polymers

Product Code 4107

2,390 Spectra

Collection of ATR reference spectra of commercially available monomers, polymers, and precursors. Contains spectra used in films, coatings, finishes, and laminates.

Basic Monomers & Polymers Database v. 1 (Unmodified)

Product Code 4219

1,490 Spectra

Collection of products selected to provide a broad base for solving polymer and plastic analytical problems. This collection includes many classic compounds, which makes it particularly useful as a reference.

Basic Monomers & Polymers Database v. 2 (Unmodified)

Product Code 4225

850 Spectra

Collection of products selected to provide a broad base for solving polymer and plastic analytical problems. This database provides additional spectra and can be used with volume one to create a comprehensive collection of basic polymeric compounds.

Coating Chemicals

Product Code 4213

720 Spectra

Collection designed to provide a convenient and practical reference source of information for chemists and technologists in the coatings industry. The database is divided into two sections: Part I - Resins and Part II - Monomers, Precursors, and Additives. It is grouped by coatings classification and arranged within each group by chemical class.

Controlled Pyrolyzates of Polymers

Product Code 4340

2,970 Spectra

This database contains the spectra of polymers which have been pyrolyzed at a constant specified temperature. It is designed to aid in the identification of the principal polymer types.

Electric Power Plant Materials

Product Code 4270

1,070 Spectra

This database contains spectra of commercial products such as seals, elastomers, polymers, lubricants, and related materials used in utility plants.

Epoxy Resins, Curing Agents, & Additives

Product Code 4363

700 Spectra

Database of FT-IR spectra that contain raw materials used in the production of thermoset materials, such as composites, printed circuit boards, and electronic packaging, as well as materials used in paints, sealants, adhesives, and a wide range of surface coatings.

Flame Retardants

Product Code 4204

590 Spectra

IR database with spectra of commercially available non-reactive and reactive flame retardants.

Hummel Defined Polymers 

Product Code 4655

2,330 Spectra

Database by Chemical Concepts. A Wiley Division. Professor Dieter O. Hummel's *Atlas of Polymer and Plastics Analysis, Volume 1, Band 1: Defined* is well known and used throughout the world. It contains spectra of polymers, copolymers, and polymer additives and can be used for quality control, characterization, or structure elucidation.

Hummel Defined Polymers, Basic Collection 

Product Code 4656

1,040 Spectra

Database by Chemical Concepts. A Wiley Division. This is a subset of the Hummel Defined Polymers database and contains polymers, copolymers, and polymer additives.

Hummel Industrial Polymers, v. 1-3 

Product Code 4651

5,000 Spectra

Database by Chemical Concepts. A Wiley Division. A collection of FT-IR spectra of polymers individually reviewed by Professor Dieter O. Hummel. These compounds are actively being used in industry and were collected directly from the manufacturers or research laboratories responsible for their development.

Hummel Industrial Polymers, v. 1 

Product Code 4652

1,910 Spectra

Database by Chemical Concepts. A Wiley Division. Collection of natural and synthetic construction polymers, natural and synthetic fibers, elastomers, miscellaneous resins like natural resins, paint and finishing resins, impregnation and casting resins, dispersion, molding and printing inks, oils, fats, waxes, tars, inorganic compounds, adhesives, putties, cements, protective colloids, curing agents, initiators and activators, accelerators, and modifiers.

Hummel Industrial Polymers, v. 2 

Product Code 4653

1,560 Spectra

Database by Chemical Concepts. A Wiley Division. One of the world's largest commercially available collections of monomers used in polymerization processes. Includes the following monomer classes: vinyl monomers, pyrolyzates, alcohols, phenols, carboxylic acids and their salts, esters, anhydrides, amides, hydrazides, urethanes, cyanates, fulminates, heterocycles, amino and thiocarboxylic acids, sulfonamides, technical solvents, and more.

Hummel Industrial Polymers, v. 3 

Product Code 4654

1,520 Spectra

Database by Chemical Concepts. A Wiley Division. Professor Hummel's enhanced polymer additives and auxiliaries FT-IR database provides a comprehensive reference source of information for polymer chemists and technologists. It includes the following classes: antioxidants, stabilizer (including PVC stabilizer), light stabilizer, coloring agents, brightening agents, fillers, plasticizers, elasticators, extenders, processing agents, textile auxiliaries, vulcanization agents, and rubber auxiliaries.

Hummel/Sadtler Polymers 

Product Code 4222

1,920 Spectra

This database is a product of a cooperative effort between Professor Dieter Hummel of the University of Cologne and Bio-Rad. It includes a wide range of polymers, copolymers, and polymer additives.

Monomers & Polymers (Comprehensive)

Product Code 3219

11,270 Spectra

World's largest commercially available collection of infrared spectra of monomers, polymers, catalysts, curing agents, antioxidants, stabilizers, modifiers, and other additives used in polymerization processes. The polymers include aliphatic hydrocarbons, polyesters, polyamides, sulfonated polymers, silicones, epoxy resins, vinyl and vinylidene polymers, cellulose derivatives and methacrylic polymers, heterocyclic vinyl polymers, and polymerized fats. It also includes a number of monomers.

Monomers & Polymers v. 1 (Modified)

Product Code 4220

1,790 Spectra

This collection contains commercial products, including additives selected to provide a broad base for solving polymer and plastic analytical problems. Product classifications include polyethylenes, polypropylenes, polystyrenes, polybutadienes, polyethers, polyacrylics, polyesters, and polyvinylpyridines. It includes many classic compounds, which makes it particularly useful as a reference. (The compounds have been selected and reviewed by Richard A. Nyquist.) The spectra are arranged into forty-nine chemical classes and have been placed in order of increasing chemical complexity within each class.

Spectral Databases

Monomers & Polymers v. 2 (Modified)

Product Code 4223

1,700 Spectra

This collection of monomers, polymers, and precursors can be used by researchers engaged in compound identification, quality control, deterioration studies, materials selection, or classroom instruction. It contains spectra of commercial products and provides a broad base for solving analytical problems in the area of polymer and plastic analysis. Product classifications include polyethylenes, polypropylenes, polystyrenes, polybutadienes, polyethers, polyacrylics, polyesters, and polyvinylpyridines. (The compounds have been selected and reviewed by Richard A. Nyquist.) Includes forty-six monomer and polymer classes.

Plasticizers

Product Code 4337

1,480 Spectra

This database contains a wide range of commercially available plasticizers that are used in the processing and compounding of polymers. A partial list of the classes of compounds which appear in the collection includes formalines, hydrocarbons, lactams, mellitates, nitriles, phenoxy, and polyesters; derivatives of acids such as abietic, adipic, benzoic, caprylic, citric, fumaric, isophthalic, lauric, maleic, oleic, palmitic, phthalic, sebacic, stearic, succinic, and tartaric; and derivatives of compounds including biphenyls, epoxy resins, ethers, ethylenediamine, glycerol, glycol, and paraffin.

Polymer Additives

Product Code 4248

1,740 Spectra

Bio-Rad has compiled a reference collection of infrared spectra of polymer additives to provide a convenient and practical reference source of information for polymer chemists and technologists.

Polymeric Compounds

Product Code 4399

470 Spectra

This database contains basic polymers commonly encountered in both industry and academia. It includes construction polymers, elastomers, miscellaneous resins, tars, inorganic compounds, curing agents, initiators and activators, accelerators, and modifiers.

Protective Materials

Product Code 4475

770 Spectra

This infrared database of polymer additives includes coatings, inhibitors, stabilizers, antioxidants, antistatic agents, and preservatives.

Rubber Chemicals

Product Code 4243

580 Spectra

The database contains the infrared spectra of rubber chemicals grouped by principal function. It includes a broad range of chemical classes used in the rubber industry, including accelerators, activators, retardants, vulcanizers, antioxidants, plasticizers, tackifiers, and stabilizers.

Sadtler/Scholl Polymer Processing Chemicals

Product Code 4232

1,150 Spectra

Collection includes polymer processing reagents such as plasticizers, inorganic fillers and pigments, organic pigments, UV stabilizers, fluorescent whitening agents, antioxidants, stabilizers, antistatic agents, biocides, flame retardants, accelerators, curing agents and activators, processing aids, and solvents. The database first appeared as Volume Three of the *Hummel/Scholl Polymer Atlas*, which is based upon data originally prepared by Dr. Friedrich Scholl.

IR Databases: Pure Organic Compounds

 Contains Structures

Alcohols & Phenols

Product Code 4381

1,920 Spectra

This database contains spectra of alcohol and phenol compounds used as solvents and in the synthesis of other compounds.

Aldehydes

Product Code 4382

690 Spectra

This database of aldehyde compounds provides access to compounds essential to the perfume and flavoring industries, as well as the manufacture of pharmaceutical intermediates and plastic additives.

Amino Acids & Peptides

Product Code 4383

790 Spectra

This database contains spectra of amino acids, peptides, and compounds with the amino acid as a unit. This collection of substances with biological importance enables users to search compounds that contain these essential building blocks.

Anhydrides & Lactones 

Product Code 4384

320 Spectra

Database of infrared spectra compiled to present compounds containing these organic compounds.

Carboxylic Acids 

Product Code 4385

1,520 Spectra

This database contains infrared spectra of acid compounds widely used in synthesis of other compounds.

Condensed Phase IR Standards (Comprehensive) 

Product Code 3201

75,570 Spectra

Comprehensive database of infrared reference spectra of organic compounds. It includes spectra of most simple aliphatic, aromatic, alicyclic, and heterocyclic compounds, as well as numerous complex materials. Numerous series of homologous compounds, ranging from the very simple to the very complex, which enable spectroscopic studies of trends involving the homologues, are also included.

Dyes, Alkynes, & Azo Compounds 

Product Code 4386

940 Spectra

This database contains spectra of dyes, alkynes, and azo compounds. It provides a reference of pure dye compounds for those in the dye or color industry.

Esters 

Product Code 4387

1,800 Spectra

This collection contains the infrared spectra of esters. The compounds are widely used in the fragrance industry, but their applications are widespread.

Explosive Materials 

Product Code 4388

720 Spectra

This database contains compounds that may be considered explosive or components of explosives. The database includes compounds mentioned in the "2002 List of Explosive Materials" produced by the Bureau of Alcohol, Tobacco, and Firearms. It also includes azide explosives, nitrate explosive mixtures, picrate explosives, peroxides, and perchlorates.

Gases & Vapors 

Product Code 4205

150 Spectra

The spectra in this database include permanent gases, as well as vapors of volatile liquids which are frequently encountered in the laboratory and in process plants. Many of the compounds included are useful in reference to atmospheric contaminant analysis relating to current air quality standards legislation, including the National Ambient Air Quality Standards Act and the Occupational Safety and Health Standards Act. The database contains the following chemicals classes: hydrocarbons, aldehydes, freons, nitrogen compounds, and sulfur compounds.

Hydrocarbons 

Product Code 4390

1,060 Spectra

This database contains infrared spectra of hydrocarbon compounds and provides a convenient reference for researchers.

Hydrocarbons & Halogenated Hydrocarbons 

Product Code 4391

1,880 Spectra

This collection includes infrared spectra of hydrocarbons and halogenated hydrocarbon compounds.

Industrial Chemicals, FT-IR Pure Organic Compounds 

Product Code 4658

20,310 Spectra

Database by Chemical Concepts. A Wiley Division. FT-IR spectral collection of organic compounds used as industrial chemicals.

Industrial Chemicals, FT-IR Basic Organic Compounds 

Product Code 4659

1,000 Spectra

Database by Chemical Concepts. A Wiley Division. Collection contains spectra of common organic compounds hand-picked from Chemical Concepts' FT-IR Organic Compounds collection.

Intermediates (Unblended) 

Product Code 4229

490 Spectra

This database contains the infrared spectra of chemicals which are intermediates in the manufacture of other end products arranged in 17 major classes of compounds. Includes acids, alcohols, aldehydes, amines, nitriles, sulfides, ketones, aromatic hydrocarbons, etc.

Spectral Databases

Ketones

Product Code 4392

1,810 Spectra

This database contains infrared spectra of ketone compounds that can be used for identification, classification, and verification of these materials.

Merck/Sadtler

Product Code 4245

2,940 Spectra

This database was prepared from the FT-IR spectra used in the *Merck FT-IR Atlas* of pure substances from the Merck-Schuchardt program.

Nucleic Acids, Nucleosides, & Nucleotides

Product Code 4393

1,450 Spectra

This database contains infrared spectra of nucleic compounds. This collection of compounds can be used for identification, classification, and verification of these materials and was compiled for those who are researching molecular processes.

Organometallics, Inorganics, Silanes, Boranes, & Deuterium Compounds

Product Code 4394

1,140 Spectra

This database of infrared spectra has been compiled specifically to present compounds containing boron, silicon, and deuterium as well as organometallics and inorganics.

Phosphorus Compounds

Product Code 4395

1,110 Spectra

This database contains infrared spectra of phosphorus compounds and can be used for identification, classification, and verification of these materials.

Q-Sadtler Reference Database

Product Code 4260

10,000 Spectra

Comprehensive database of pure organics commonly found in both academic and industrial laboratories covering a broad range of chemical classes from commercially available sources. It is frequently used in organic chemistry and other college courses to establish chemical identity through comparison of functional groups. This database can also be used as a reference for industrial laboratories to identify organic compounds using infrared spectroscopy.

Selected IR Reference Database

Product Code 4000

2,500 Spectra

This database contains pure organic chemicals, which can be used to identify and classify pure samples and can serve as a reference when more comprehensive collections are not available.

Select Standards

Product Code 4202

2,490 Spectra

This database contains spectra representing a broad range of both simple and complex pure compounds. It was designed to satisfy the need for a small, convenient collection of infrared spectra of organic compounds when more comprehensive collections are not available.

Select Vapor Phase

Product Code 4228

500 Spectra

IR database with vapor phase spectra to accompany Nyquist's *The Interpretation of Vapor Phase Infrared Spectra - Group Frequency Data*. It provides a basic collection of compounds analyzed using the vapor phase technique.

Solvents (Unblended)

Product Code 4360

630 Spectra

This database contains the FT-IR reference spectra of common solvents to aid in identification and analysis of these compounds.

Solvents by ATR FT-IR

Product Code 4361

620 Spectra

Database contains ATR FT-IR reference spectra of common solvents using standard attenuated total reflectance techniques.

Solvents by Vapor Phase

Product Code 4362

620 Spectra

Database contains FT-IR reference spectra of common solvents. Spectroscopists identifying compounds in the vapor state from gas chromatography separations will find this database very useful.

Starter Databases **Product Code 4050****11,800 Spectra**

The Sadtler Starter Database is a collection of infrared reference spectra, including organic chemicals and trade name monomer and polymer compounds.

Steroids Database **Product Code 4396****860 Spectra**

This database contains FT-IR spectra representing important classes of compounds to steroid research.

Sugars & Carbohydrates **Product Code 4397****570 Spectra**

This database contains infrared spectra of sugars and carbohydrates and is useful for identification, classification, and verification of these materials. Carbohydrates contain a broad range of sugars, starches, and fibers.

Sulfur Compounds **Product Code 4398****1,090 Spectra**

This database contains infrared spectra of sulfur compounds and is useful for identification, classification, and verification of these materials.

University Standards **Product Code 4201****300 Spectra**

This database provides a small convenient collection of infrared spectra of organic compounds relevant to college introductory courses on organic chemistry and supplementary laboratory courses on experimental organic chemistry and qualitative organic analysis. They are arranged by chemical class.

Vapor Phase IR Standards (Comprehensive) **Product Code 3203****9,190 Spectra**

Collection includes IR vapor phase spectra of common pure organic compounds to identify unknown compounds by GC-IR, TGA-IR, or other vapor phase methods of analysis. The compounds are critical to pollution and toxicological identification.

IR Databases: Industrial Compounds**Basic Surfactants (Unmodified)****Product Code 4367****850 Spectra**

This collection provides scientists working with surface active agents a reference database of representative compounds. Contains FT-IR spectra of anionic, cationic, and nonionic compounds.

Fats, Waxes, & Derivatives**Product Code 4325****1,800 Spectra**

Compounds in this database include animal fats and oils, animal waxes (raw and refined), fatty acids, fatty acid esters (other than triglycerides), fatty amides, fatty amines, unsaponifiable matter, other fatty derivatives, marine fats and oils, mineral waxes (crude and refined), modified mineral waxes, modified vegetable waxes, synthetic waxes, soaps, vegetable fats and oils, and vegetable waxes (raw and refined).

Hummel Surfactants**Product Code 4657****1,030 Spectra**

Database by Chemical Concepts. A Wiley Division. This database contains spectra of surfactants compiled by Professor Dieter O. Hummel. In order to present a comprehensive database of compounds for those using surfactants, research samples and industrial surfactants were used to create the data.

Intermediates (Industrial Quality)**Product Code 4329****830 Spectra**

IR database with spectra of commercially available chemicals used as precursors to desired end-products, including acids, alcohols, aldehydes, amines, ketones, nitriles, sulfides, and aromatic hydrocarbons. These compounds are used to manufacture products such as pharmaceuticals, surfactants, dyes, plasticizers, and other specialty chemicals.

Spectral Databases

Lubricants

Product Code 4217

880 Spectra

This database contains infrared spectra of commercially available compounds used in a variety of industrial and automotive applications that perform these functions such as greases, hydraulic fluids, cutting oils, motor oils and metallic soaps. Included are products of petroleum origin and synthetic lubricants such as chlorofluorocarbons (CFCs), dibasic carboxylic acid esters, lubricating polymers, phosphate esters, and silicones.

Lubricant Additives

Product Code 4255

1,570 Spectra

A collection of additives used in engine oils, transmission and hydraulic fluids, gear oils, industrial oils, metalworking, and process oils. They are used in the automotive, marine, aeronautic, and petroleum industries, as well as any industry that makes use of machinery. The spectra have been run heavier than usual to compensate for the nature of the compounds.

Petroleum Chemicals

Product Code 4208

320 Spectra

These spectra are of compounds chosen from commercially available petroleum products, many of which are used in modifying and improving gasolines, fuel oils, lubricants, and other products. Some of the more than 20 classes represented in this database include antiacids, antidetonants, antioxidants, catalysts, dispersants, gum inhibitors, gum solvents, ignition control compounds, rust preventatives, viscosity improvers, etc.

Polyols

Product Code 4226

270 Spectra

This database contains infrared spectra of commercially available polyols. It includes polyols, polyglycols, glycerols, carbohydrates, starches, mono-, di-, and polysaccharides used as lubricants, prepolymers, and intermediates in the manufacture of drugs and many industrial products.

Solvents (Industrial Quality)

Product Code 4327

910 Spectra

This database provides a convenient, practical reference that aids in identification and analysis of common industrial solvents. The solvents are classified into four main groups: hydrocarbons, compounds having only one type of characteristic atom or functional group, compounds having more than one type of characteristic atom or functional group, and deuterated compounds.

Surfactants (Comprehensive)

Product Code 3235

10,000 Spectra

The largest commercially available collection of infrared spectra of detergents, emulsifiers, defoamers, softeners, sequestering agents, soaps, builders, and formulating products.

Surfactants v. 1 (Modified)

Product Code 4235

1,790 Spectra

Collection of IR spectra selected to assist in solving analytical problems in the area of surfactant analysis. Analytical applications include identification, quality control, decomposition studies, product selection, in-situ study of their particular utility, plus other uses such as academic instruction. The collection consists of commercially available products such as soaps, emulsifiers, chelating agents, corrosion inhibitors, slip agents, thickening agents, optical bleaches, lubricants, defoamers, sequestering agents, softeners, etc.

Surfactants v. 2 (Modified)

Product Code 4252

1,700 Spectra

This collection of IR spectra selected to assist in solving analytical problems in the area of surfactant analysis. These products are utilized as detergents, soaps, emulsifiers, chelating agents, corrosion inhibitors, slip agents, thickening agents, optical bleaches, lubricants, etc.

IR Databases: Forensic Sciences

 Contains Structures

ATR of Controlled & Prescription Drugs

Product Code 4479

1,160 Spectra

This database contains ATR-IR spectra of controlled and prescription drugs as well as steroids that may be of interest to forensic laboratories or any researcher analyzing drug samples.

ATR of Steroids, Androgens, Progestins, & Estrogens

Product Code 4478

300 Spectra

The database, prepared by Forensic Spectral Research, contains steroids, androgens, progestins, and estrogens useful in forensic, pharmaceutical, medical, and other applications.

Automobile Paint Chips

Product Code 4603

1,990 Spectra

This collection is intended primarily for use in making color comparisons and/or chemical comparisons. All the color chips in the database were prepared from actual production paint batches. Paint types included are acrylic solution lacquer, acrylic dispersion lacquer, acrylic enamel, polyester enamel, urethane enamel, base coat/clear coat acrylic enamel, non-aqueous dispersion enamel (NAD), water-based enamel, etc.

Biochemicals 

Product Code 4472

590 Spectra

This database contains infrared spectra of a variety of biochemicals such as peptides, amino acids, carbohydrates, nucleic acids, sugars, lipids, steroids, terpenes, alkaloids, glycosides, carotenoids, flavonoids, etc.

Canadian Forensics

Product Code 4212

3,490 Spectra

This database contains spectra of legal and illegal drugs, drug precursors, and the reagents used to prepare them, as well as other substances encountered in forensic analysis. Some common laboratory and household reagents have been included as well. This database was produced by the Department of National Health and Welfare of the Government of Canada.

Commonly Abused Drugs (Acid/Base)

Product Code 4214

580 Spectra

This collection contains spectral data on drugs which are frequently misused. The compounds represented are predominately brand name drugs in dosage form with some drugs in bulk supply form and some narcotics. Some mixtures in this collection are street drugs, that is, mixtures of narcotics that have been unlawfully prepared.

Dyes 

Product Code 4216

520 Spectra

This collection of dyes provides a convenient and practical reference source of information for chemists and technologists in the dye or color industry. Dyes are grouped into classes based on usage established by the Colour Index (C.I.).

Dyes, Pigments, & Stains

Product Code 4316

2,550 Spectra

This collection of dyes, pigments, and stains provides a convenient and practical reference source of information for chemists and technologists in the dye industry.

Fibers & Textile Chemicals

Product Code 4203

480 Spectra

Collection contains natural and synthetic fibers from domestic and foreign sources. Among the natural fibers represented are: silk, wool, cotton, kapok, flax, jute, hemp, sisal, raffia, and asbestos. Synthetic fibers include all generic classifications defined in the Textile Fiber Products Identification Act (with the exception of metallic class). Classes include acetate, acrylic, nylon, nylril, polyester, rayon, triacetate, vinyl, and vinylon. Textile chemicals include defoamers, detergents, bleaches, antistats, conditioners, finishers, softeners, and other agents.

Fibers by Microscope

Product Code 4364

450 Spectra

This database contains high-quality reference spectra of commercially available synthetic fibers measured by FT-IR instrument and microscope. The spectra were measured on fiber and yarn samples, and multiple spectra are provided for two or more components in a yarn.

Flavors, Fragrances, & Oils 

Product Code 4365

870 Spectra

This database provides scientists with a representative collection of organic compounds used in the manufacture of flavors and fragrances, natural product oils, synthesized fragrance compounds, terpenes, and some fixatives. The database includes infrared spectra of compounds that are approved by the Flavor and Extracts Manufacturers' Association of the United States.

Flavors & Fragrances (IR Vapor Phase) 

Product Code 4474

490 Spectra

IR database with vapor phase spectra of pure organic compounds used in the manufacture of flavors, fragrances, and synthesized compounds.

Food Additives 

Product Code 4671

990 Spectra

IR database with spectra of ingredients added directly to food that FDA has either approved as food additives or listed or affirmed as GRAS.

Spectral Databases

Georgia State Crime Lab

Product Code 4604

1,910 Spectra

Collection of infrared reference spectra of controlled substances as well as compounds likely to be encountered in routine analysis and used for the instrumental analysis of drugs prepared at the Division of Forensic Sciences, Georgia State Crime Laboratory, Atlanta, Georgia.

Pharmaceutical Excipients

Product Code 4471

880 Spectra

This database was prepared for those studying pharmaceutical formulations using infrared spectroscopy and it contains spectra of materials used in the development, production, control and regulation of pharmaceutical preparations. These compounds may be classified as binders, fillers, diluents, flow enhancers, sweeteners, coatings, preservatives, dispersing agents, flavors, suspending agents, compression aids, etc.

Pharmaceuticals

Product Code 4431

560 Spectra

Comprehensive collection of drugs, medicinals, and pharmaceutical preparations frequently encountered in medical and pharmaceutical research and drug analysis. Compounds have been selected from: *Modern Drug Encyclopedia*, *The U.S. Pharmacopoeia*, *The British Pharmacopoeia*, *The International Pharmacopoeia*, *New and Non-Official Drugs*, and *the National Formulary*. The classes include anesthetics, antimicrobials, antibiotics, anticoagulants, antivirals, cardiovascular agents, diuretics, enzymes, estrogens, hormones, relaxants, sedatives, stimulants, tranquilizers, and vitamins.

Prepared & Prescription Drugs (Acid/Base)

Product Code 4457

880 Spectra

This collection contains the spectra of trade name prepared and prescription drugs selected from the *Physician's Desk Reference to Pharmaceutical Specialties and Biologicals* to provide a rapid method of characterizing drugs.

Steroids

Product Code 4209

250 Spectra

This database contains FT-IR spectra representing important classes of compounds for steroid research.

Steroids, Androgens, Progestins, & Estrogens

Product Code 4477

300 Spectra

The database, prepared by Forensic Spectral Research, contains steroids, androgens, progestins, and estrogens useful in forensic, pharmaceutical, medical, and other applications.

IR Databases: Environmental Applications

 Contains Structures

HAZMAT Database

Product Code 4389

410 Spectra

Database contains infrared spectra of hazardous compounds. This collection of selected substances can be used for identification, classification, and verification of these materials.

Pesticides & Agricultural Chemicals

Product Code 4366

1,020 Spectra

Comprehensive selection of chemical materials used in all phases of agriculture. Materials in this database may also be considered industrial wastes. These compounds, most of which are pesticides, come from a variety of sources. All of the chemicals are commercially available, but this database also contains high-purity pesticide reference standards supplied to Bio-Rad by the U.S. Environmental Protection Agency. In most cases, the compounds represent the active ingredient of commercial formulations, although some complete formulations have also been included. Includes: acaricides, bactericides, nematocides, growth regulators, hormones, preservatives, nutrients, fungicides, herbicides, insecticides, repellents and attractants, miticides, rodenticides, and other agricultural chemicals.

Pollutants (IR Vapor Phase)

Product Code 4473

910 Spectra

This database provides a spectral reference for those who analyze, monitor, control, or study environmental, physiological, or occupational pollutants and toxic substances. It contains vapor phase spectra that are representative of those one would obtain using GC/FT-IR analysis where the spectra are measured above ambient temperature in a heated optical cell.

Priority Pollutants 

Product Code 4470

470 Spectra

This database is a convenient and practical spectral reference for research, industry, and all others who are engaged in analyzing, monitoring, controlling, or studying environmental, physiological, or occupational pollutants and toxic substances. These compounds have appeared in the "EPA Priority Pollutants List," the "Occupational Safety and Health Administration (OSHA) Category 1 List of Carcinogenic Substances," and a list of hazardous compounds common to industry and of concern during interstate transportation and appear on the "EPA Priority Pollutant List." The database includes compounds that are represented by two types of spectra, infrared condensed phase and infrared vapor phase.

Sadtler EPA Vapor Phase 

Product Code 4610

3,240 Spectra

The purpose of this database is to provide reference spectra pertinent to pollution and toxicological identification and contracted for this database. It includes IR vapor phase spectra of common pure organic compounds and is helpful in identifying unknown compounds by GC-IR, TGA-IR, or other vapor phase methods of analysis.

Water Treatment Chemicals

Product Code 4210

290 Spectra

Collection of infrared spectra of commercially available materials used in water treatment processes, such as boiler water additives and cooling water additives. Includes biocides, chelating agents, coagulants, and flocculating agents.

IR Databases: Inorganics & Organometallics Contains Structures**ATR of Inorganics**

Product Code 4486

260 Spectra

ATR database with spectra of inorganic compounds. The spectra are representative of many anions and polyatomic ions common to inorganic materials.

ATR of Organometallics 

Product Code 4487

170 Spectra

ATR database compiled specifically for scientists interested in organometallic chemistry. Samples have been solicited from industrial concerns and academic and research institutions in an attempt to select a cross section of compounds of interest.

Inorganics

Product Code 4359

1,100 Spectra

IR database with spectra of inorganic compounds. The spectra are representative of many anions and polyatomic ions common to inorganic materials and are classified according to anion or polyatomic ion following groups in the periodic chart. This collection contains the spectra of "classical" inorganic compounds such as ammonium sulfate, ammonium nitrate, zirconium sulfate, and coordination compounds of various metals with inorganic and organic ligands. The classes represented in this collection include inorganic compounds, inorganic coordination compounds, organic coordination compounds, metal carbonyl compounds, and boranes.

Inorganics (Subset A)

Product Code 4459

240 Spectra

IR database of inorganic compounds. The spectra are representative of many anions and polyatomic ions common to inorganic materials and are classified according to anion or polyatomic ion following groups in the periodic chart.

Minerals & Clays

Product Code 4206

420 Spectra

IR database with spectra of minerals and clays. The spectra are classified according to an increasing order of complexity of the mineral.

Organometallics 

Product Code 4207

350 Spectra

IR database compiled specifically for scientists interested in organometallic chemistry. Samples have been solicited from industrial concerns and academic and research institutions in an attempt to select a cross section of compounds of interest. This database is comprised of spectra of compounds which possess a direct carbon-to-metal bond and compounds in which the metal atom is bonded to carbon by a single hetero atom.

Spectral Databases

Raman Databases

 Contains Structures

Raman of Basic Monomers & Polymers (*Unmodified*)

Product Code 4701

1,680 Spectra

This database provides scientists with a central source of reliable polymeric data. Monomer and polymer compounds included in this collection were selected to provide simple compounds of representative functional groups for identification and classification. The database contains reference spectra, which have not been modified with any additives, although they may be copolymers or terpolymers.

Raman of Inorganics

Product Code 4702

1,630 Spectra

Inorganic compounds included in this collection were selected to provide representative materials for identification and classification. The analytical applications of this database include identification, quality control, deterioration studies, materials selection, elucidation of molecular structure, plus other applications such as process control.

Near IR Database

 Contains Structures

Near Infrared Spectra Collection of Common Organic Compounds

Product Code 4660

3,800 Spectra

Database by Chemical Concepts. A Wiley Division. Collection contains common organic compounds. The spectra were analyzed using the near infrared technique. There are two spectra per structure.

NMR Databases

NMR Metabolites Database

Product Code 8786

1,050 Spectra

A collection of ^1H and ^{13}C NMR spectra of metabolites for identifying potential biomarkers of metabolomics experiments. Data is available from the Biological Magnetic Resonance (BMRB) laboratory at the University of Wisconsin, Madison. Includes links to PubChem, KEGG, and ChEBI databases, as well as KEGG pathway displays.

^{13}C NMR of Monomers & Polymers

Product Code 8723

740 Spectra

Bio-Rad offers a database that can be used by polymer chemists and spectroscopists who study monomers, polymers, and resins using the ^{13}C NMR technique. Numerous polymer and monomer classifications are represented.

Additional Databases

Bio-Rad offers the complete line of Wiley Mass Spectral Databases:

- Wiley Registry® 9th Edition
- Mass Spectral & GC Data of Drugs, Poisons, Pesticides, Pollutants, & their Metabolites
- Mass Spectra of Designer Drugs
- Mass Spectra of Pharmaceuticals & Agrochemicals
- Mass Spectra of Androgens, Estrogens, & Other Steroids
- Mass Spectra of Organic Compounds
- Mass Spectra of Geochemicals, Petrochemicals, & Biomarkers
- FFNSC 1.3 - Flavors & Fragrances of Natural & Synthetic Compounds

Bio-Rad offers an additional proton NMR database from Wiley:

- Wiley ^1H NMR Spectra of Organic Compounds - 104,489 spectra

HaveltAll® Annual License for Databases

Bio-Rad's HaveltAll Spectral Databases allow users to search Bio-Rad's entire collections of spectra by technique. HaveltAll collections are based on an annual license. They are accessible from the KnowItAll Informatics System software or via the Internet.

HaveltAll IR

Product Code 8910

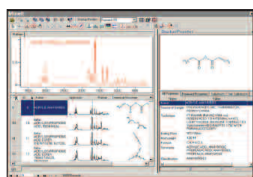


Infrared spectral collection of almost 230,000 spectra of pure organic and commercial compounds. This database is extremely useful when trying to identify or classify unknown spectra. Whether the need is to access polymers, pure organics, inorganics, organometallics, or industrial compounds within application areas such as pharmaceuticals, forensics, material sciences, and academia, users can be sure that this collection will meet their needs. Search by spectra, peak, name, structure, substructure, and property fields, such as technique, molecular weight, CAS Registry Number, etc.

Please visit www.knowitall.com/haveitallir

HaveltAll Raman

Product Code 8940

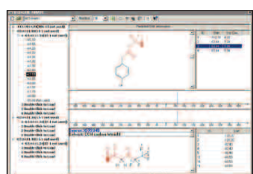


High-quality Raman data that focuses on monomers, polymers, organic, and inorganic compounds. Users can import their own spectra and search against a reference database containing 4,465 spectra. Search by spectra, peak, name, structure, substructure, and property fields, such as technique, molecular weight, CAS Registry Number, etc.

Please visit www.knowitall.com/haveitallraman

HaveltAll NMR

Product Code 8920

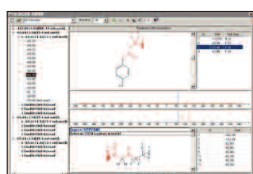


Access over 438,000 ^{13}C NMR and over 50,000 ^1H NMR reference spectra for reliable NMR predictions. Within KnowItAll's PredictIt NMR, not only can one retrieve the spectral data used to build predictions, but can also access all of the available information related to the reference spectrum, such as sample source, solvent, conditions of production, equipment, and properties for the molecule.

Please visit www.knowitall.com/haveitallnmr

HaveltAll XNMR

Product Code 8960

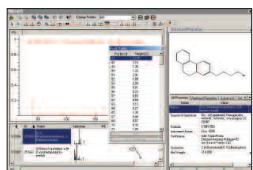


Access over 71,000 reference XNMR spectra for reliable predictions. It includes ^{19}F NMR, ^{31}P NMR, ^{15}N NMR, ^{11}B NMR, ^{17}O NMR, ^{29}Si NMR, and other nuclei. Within KnowItAll's PredictIt NMR, not only can one retrieve the spectral data used to build predictions, but can also access all of the available information related to the reference spectrum, such as sample source, solvent, conditions of production, equipment, and properties for the molecule.

Please visit www.knowitall.com/haveitallxnmr

HaveltAll MS

Product Code 8930

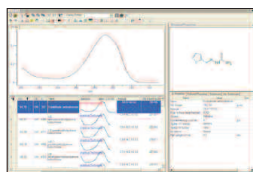


This collection of spectra and related information includes data from the National Institute of Standards and Technology (NIST) with the assistance of expert advisors from the Environmental Protection Agency (EPA) and National Institutes of Health (NIH). Search by peak, name, structure, substructure, and property fields, such as technique, molecular weight, CAS Registry Number, etc. Database also includes chemical synonyms.

Please visit www.knowitall.com/haveitallms

HaveltAll UV-Vis

Product Code 8763



This reference database is extremely useful when trying to identify or classify unknown UV-Vis spectra. Applications include pharmaceutical, forensic, environmental, materials sciences, polymers, and many others. Search by spectra, peak, name, structure, substructure and property fields, such as formula, molecular weight, solvent, concentration, and path length. Peak tables contains the position of the peak, the height of the peak, the absorption and the extinction coefficient.

Please visit www.knowitall.com/haveitalluv-vis

KnowItAll[®] Informatics System

Bio-Rad's award-winning KnowItAll Informatics System offers fully integrated software solutions that provide multiple tools for spectroscopy—all within a single user interface—including:

- Spectral Processing, Search, Analysis, & Prediction
- Result Reporting
- Database Building & Management
- Chemometrics Tools
- Chemical Structure Incorporation

True Integration.

Instantly transfer data from one application to another.

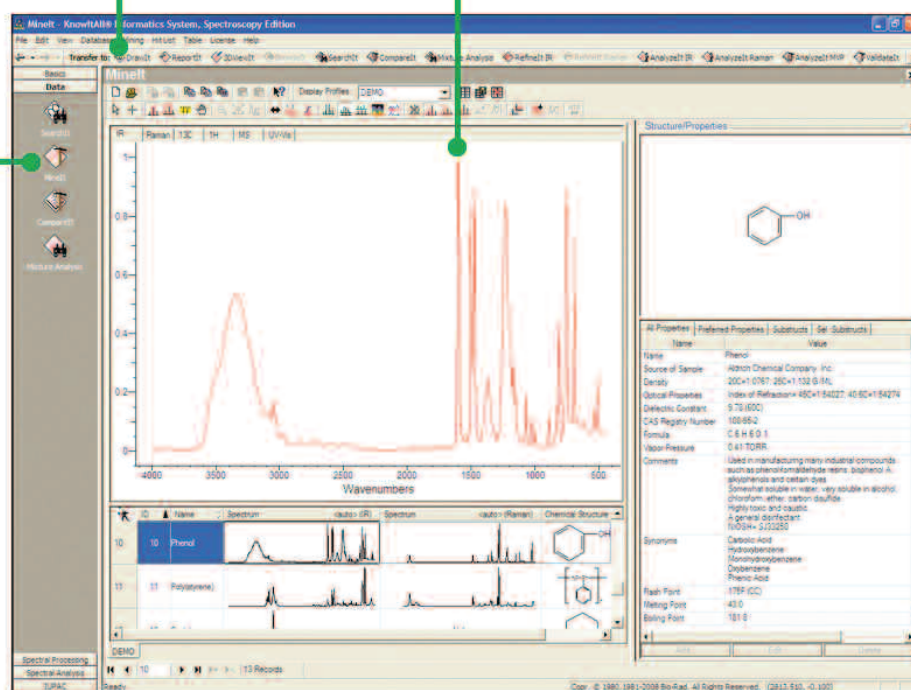
Integrated Informatics.

Search, manage, and analyze spectroscopic and chemical information.

Versatile Toolboxes.

Evaluate spectra with suite of software tools.

Desktop & Enterprise Solutions.



How the KnowItAll Interface Works

The KnowItAll interface is designed so the user can transfer information from one tool to another, and move from one task to the next, without having to leave the main interface or open another program.

Multiple tasks are performed using logically grouped "toolboxes." Because all the tools are located in a single, integrated environment, using this system will invariably save time and improve workflow.

Ultimately, by combining tools and data into one system, the end result is greater ability to extract knowledge from data.

Bio-Rad offers the following specialized "editions" of its KnowItAll system for various spectroscopic techniques. See "KnowItAll Edition Feature Comparison Chart" on page 20 for more details.

KnowItAll IR/NIR Edition

Product Code 8791



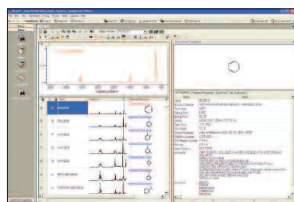
Techniques: IR, NIR

The KnowItAll IR/NIR Edition offers a fully integrated software environment for IR and NIR with data management (*optional*), spectral search, processing, structure drawing, and reporting tools. Now with unique tools for analysis such as Overlap Density Heatmaps and Spectral Mixture Analysis.

For more details and to view demo movies, please visit www.knowitall.com/iredition

KnowItAll Spectroscopy Edition

Product Code 8764



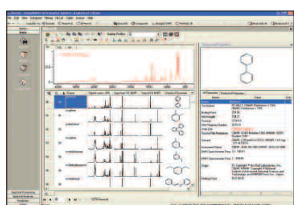
Techniques: IR, Raman, NIR, MS, UV-Vis, Chromatography

The KnowItAll Spectroscopy Edition offers a fully integrated software environment for IR, Raman, NIR, MS, UV-Vis, and chromatography that includes data management, spectral searching, processing, structure drawing, and reporting tools. Now with unique tools for analysis: Overlap Density Heatmaps and Spectral Mixture Analysis.

For more details and to view demo movies, please visit www.knowitall.com/spectroscopyedition

KnowItAll Analytical Edition

Product Code 8902



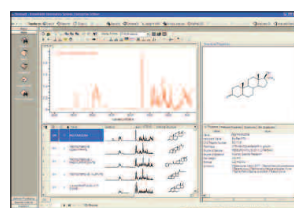
Techniques: IR, Raman, NIR, NMR, MS, UV-Vis, Chromatography

The KnowItAll Analytical Edition offers the first, fully integrated software environment for analytical techniques, including IR, Raman, NIR, NMR, MS, UV-Vis, and chromatography that includes multi-technique database management, spectral search, processing, structure drawing, and reporting tools. Now with unique tools for analysis: Overlap Density Heatmaps and Spectral Mixture Analysis. Includes additional mass spec filters.

For more details and to view demo movies, please visit www.knowitall.com/analyticaledition

KnowItAll Enterprise Edition

Product Code 8794



Techniques: IR, Raman, NIR, NMR, MS, UV-Vis, Chromatography

The award-winning KnowItAll Enterprise Edition offers the first, fully integrated software environment for analytical techniques, including IR, Raman, NIR, NMR, MS, UV-Vis, and chromatography that includes multi-technique database management (*optional*), spectral search, processing, structure drawing, and reporting tools. Now with unique tools for analysis: Overlap Density Heatmaps and Spectral Mixture Analysis.

KnowItAll Raman Edition

Product Code 8907



Technique: Raman

The KnowItAll Raman Edition offers a fully integrated software environment for Raman spectroscopy with data management (*optional*), spectral searching, processing, structure drawing, and reporting tools. Now with unique tools for analysis such as: Overlap Density Heatmaps and Spectral Mixture Analysis.

For more details and to view demo movies, please visit www.knowitall.com/ramanedition

KnowItAll UV-Vis Edition

Product Code 8765



Technique: UV-Vis

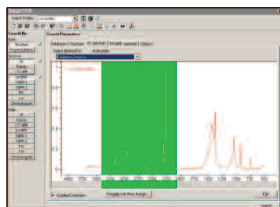
The KnowItAll UV-Vis Edition offers a fully integrated software environment for UV-Vis that includes data management, spectral searching, structure drawing, and reporting tools. Now with unique tools for analysis: Overlap Density Heatmaps and Spectral Mixture Analysis.

For more details and to view demo movies, please visit www.knowitall.com/uv-visedition

KnowItAll Software Features

Included Applications & Features

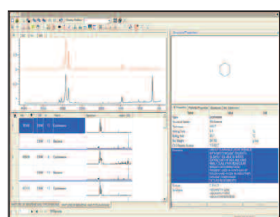
SearchIt™ - Database Searching *(full spectrum, structure, peak, property, etc.)*



The SearchIt application allows structures and/or spectra to be imported and searched against licensed reference databases, as well as against KnowItAll user-created databases. Searches are fully customizable and are driven by state-of-the-art algorithms. Searching can be performed by structure, substructure, name, properties, spectra, or any combination.

For more details and to view demo movies, please visit www.knowitall.com/searchit

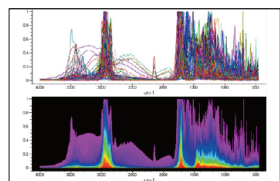
Spectral Mixture Analysis - Analyze Experimental Spectral Data of Mixtures



This application deconvolutes components of a mixture by analyzing a spectrum. It allows comparison of a sample spectrum against KnowItAll databases of a user's own proprietary spectra as well as any licensed KnowItAll reference databases. 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 (the difference between the query spectrum of the actual mixture and the composite spectrum). The composite spectra are ranked by how closely they resemble the query spectrum.

For more details and to view demo movies, please visit www.knowitall.com/mixtureanalysis

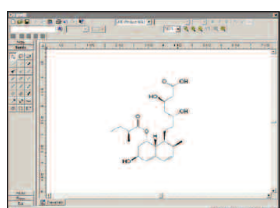
Overlap Density Heatmaps - Visual Data Mining and Analysis



Bio-Rad has introduced a breakthrough technology for visual data mining and analysis to assess the similarities and dissimilarities in massive amounts of spectral, chromatographic, or other graphical data.† This patented technology, called Overlap Density (OD) Heatmaps displays allows scientists to visualize the common features of the overlapped objects (such as spectra or chromatograms) by color coding.

For more details and to view demo movies, please visit www.knowitall.com/odhm

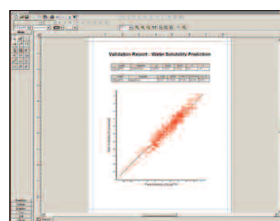
DrawIt™ (ChemWindow®) - 2D Structure Drawing *(includes stereochemical recognition)*



With DrawIt, users can draw any chemical structure with just a few clicks and drags. It has all the tools users need to draw rings, bonds, atoms, chains, arrows, and chemical symbols.

For more details and to view demo movies, please visit www.knowitall.com/drawit

ReportIt™ - Custom Publishing Tools



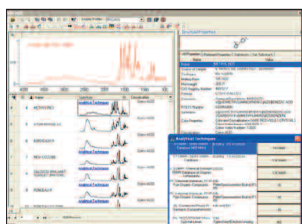
With ReportIt, users can create standard reports, presentations, and publications. Reports are easy to lay out by using one of our predefined or custom templates.

For more details and to view demo movies, please visit www.knowitall.com/reportit

Optional Applications & Features

Database Building Option - Build Databases with Spectra, Structures, & Properties

Product Code 8501



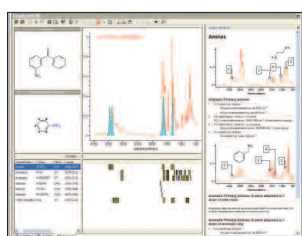
Chemists and spectroscopists produce valuable data every day within their organizations. With KnowItAll's Minelt Database Building option, researchers can capture these resources and build searchable databases that include multiple analytical techniques† (IR, Raman, NIR, NMR, MS, UV-Vis, chromatography), chemical structures, and alphanumeric data.

For more details and to view demo movies, please visit www.knowitall.com/databasebuilding

(Included in Spectroscopy, Analytical, Enterprise, and UV-Vis but optional in other KnowItAll editions)

AnalyzeIt™ IR - Functional Group Analysis

Product Code 8512

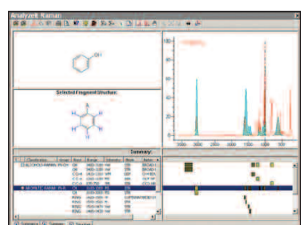


AnalyzeIt IR can be used to help interpret the bands in an infrared spectrum. Simply load a spectrum and click on a peak of interest to generate a list of all function groups possible at that position. AnalyzeIt also suggests the best peak to begin interpretation. It features over 200 function groups and hundreds of interpretation frequencies. The application also allows correlation from a structure. Now users can link to additional reference information for each functional group in the *Sadtler Handbook of Reference Spectra - IR*. Users can also build their own knowledgebase of functional groups that can be used in the interpretation.

For more details and to view demo movies, please visit www.knowitall.com/analyzeitir

AnalyzeIt Raman - Functional Group Analysis

Product Code 8942

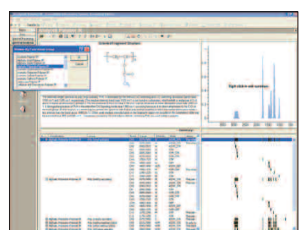


AnalyzeIt Raman can be used to help interpret the bands in a Raman spectrum. Simply load a spectrum and click on a peak of interest to generate a list of all functional groups possible at that position. AnalyzeIt also suggests the best peak to begin interpretation. It features over 200 functional groups and hundreds of interpretation frequencies. The application also allows correlation from a structure. Users can also build their own knowledgebase of functional groups that can be used in the interpretation.

For more details and to view demo movies, please visit www.knowitall.com/analyzeitraman

AnalyzeIt Polymer IR - Polymer Analysis

Product Code 8547

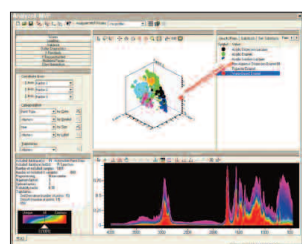


The identification, classification, and interpretation of commercial polymers is challenging. A key piece of desired information is the spectral-structure correlation information not available from spectral searching alone. AnalyzeIt Polymer IR—in tandem with a knowledge base of polymer spectral-structure correlations—is an application developed specifically to assist in this process. Users can also build their own knowledgebase of functional groups that can be used in the interpretation.

For more details and to view demo movies, please visit www.knowitall.com/analyzeitpolymerir

AnalyzeIt MVP - Multivariate Processing

Product Code 8508



AnalyzeIt MVP, which incorporates Infometrix' chemometrics technology for principal component analysis (from the well-known Pirouette® software) of spectroscopic, chromatographic, or numeric data,† enables a user to:

- Gain insight into hidden patterns and relationships in users' data
- Explore data correlations to answer critical research, development, or production questions
- Store results for subsequent reference, reporting, or investigation

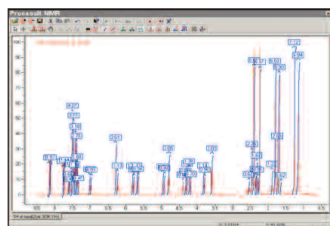
For more details and to view demo movies, please visit www.knowitall.com/analyzeitmvp

KnowItAll Software Features

Optional Applications & Features

ProcessIt™ NMR - NMR Spectrum Processing

Product Code 8926



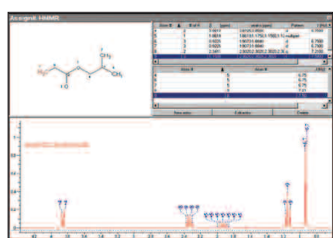
This feature allows users to import and process NMR signal or spectra from various formats. With this application, one can execute multiple-step processing either step-by-step or by using a macro capability to accomplish in batch mode.

For more details and to view demo movies, please visit www.knowitall.com/processitnmr

(Included in the Analytical and Enterprise editions)

AssignIt™ NMR - Add Assignments to NMR Databases

Product Code 8927

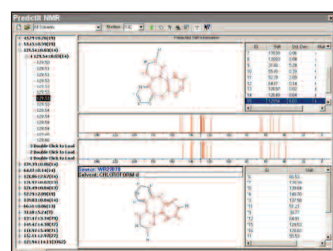


With this tool, add assignments and other information to structures in ^1H , ^{13}C , ^{19}F , ^{31}P , ^{15}N , ^{17}O , ^{11}B , and ^{29}Si KnowItAll NMR databases. AssignIt allows quick information input, such as peak shift assignments, intensities, coupling constants, multiplicities, and links to the relevant chemical structure or proposed structure.

For more details and to view demo movies, please visit www.knowitall.com/assignit

(Included in the Analytical and Enterprise editions)

PredictIt™ NMR - NMR Spectrum Prediction



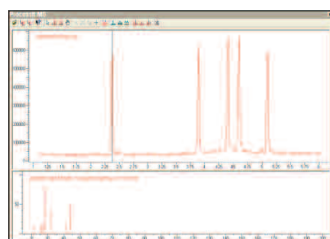
With the PredictIt NMR application, database-based NMR spectrum predictions can be performed for ^{13}C , ^1H , and many other nuclei. Predictions occur automatically when users open a structure in the application. To make predictions, KnowItAll examines any licensed databases of substructures that have ^1H , ^{13}C , or other shifts assigned to them. The substructures are defined by the number of shells that represent atoms within "n" bonds of the central atom.

For more details and to view demo movies, please visit www.knowitall.com/predictitnmr

(Included in the Analytical and Enterprise editions)

ProcessIt MS - MS & Hyphenated MS Processing

Product Code 8547



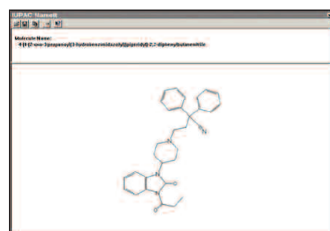
The ProcessIt MS application can be used to import and open GC/MS and LC/MS files and view and select MS scans within them. Selected MS scans can be added to user databases and can be searched. In addition, this application enables users to perform spectral averaging and subtraction and allows the display of selected ion chromatograms (SICs).

For more details and to view demo movies, please visit www.knowitall.com/processitms

(Included in the Spectroscopy, Analytical, and Enterprise editions)

IUPAC NameIt™ & DrawIt - Systematic IUPAC Names from Structures & Vice Versa

Product Code 8544



With KnowItAll's IUPAC NameIt and IUPAC DrawIt options, effortlessly name or create structures using systematic IUPAC rules. Simply enter a structure or a name, click a button, and generate the corresponding name or structure based on internationally accepted standard nomenclature rules—without having to memorize them. Generating names and structures this way not only saves time, but also ensures accuracy and standardization of communication and data mining within the laboratory.

For more details and to view demo movies, please visit www.knowitall.com/iupac

Optional Applications & Features

Infometrix' Pirouette® Software - Chemometrics Tools for Classification, Data Exploration, & More

Prediction, classification, data exploration and multivariate regression methods are implemented in this chemometrics software from Infometrix, which now includes mixture analysis. A simple to use, yet very powerful interface, facilitates interacting with raw and processed data. Support for many common instrument and data exchange file formats make importing data painless. Thousands of subsets can be created from a single data file, allowing the user to exercise many different "what-if" scenarios without having to collect additional data.

For more details, please visit www.knowitall.com/pirouette

PhysChem Predictive Modules - Choose from Log D, Log P, Water Solubility, pKa, etc.

Bio-Rad offers PhysChem and ADME predictive models for use with certain editions of the KnowItAll Informatics System.

For more details, please visit www.knowitall.com/physchem

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 HaveItAll 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	○	○	○	○	○	○
PhysChem Modules	Choose from many models including Log D, Log P, Solubility, pKa, etc.	○	○	○	○	○	○

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.

IR

Sadtler IRF (*.irf)	Generic XY Data (*.*)	Mattson (*.ras, *.abs)
Bomem (*.a01)	Horiba MDW (*.mdw)	PE Spectrum (*.sp)
Bruker (*.*)	JASCO (*.jws, *.j1d)	Shimadzu (*.irs, *.smf)
Digilab (*.dt)	JCAMP (*.dx, *.jdx)	Spectacle/Shimadzu (*.irs)
Galactic/GRAMS (*.spc, *.fir, *.ir, *.rmn)	JEOL (*.wsf)	Thermo/Nicolet (*.spa)

Raman

Sadtler IRF (*.irf)	Horiba MDW (*.mdw)	PE Spectrum (*.sp)
Bomem (*.a01)	JASCO (*.jws, *.j1d)	Renishaw WIREF (*.wxd)
Bruker (*.*)	JCAMP (*.dx, *.jdx)	Shimadzu (*.irs, *.smf)
Digilab (*.dt)	JEOL (*.wsf)	Spectacle/Shimadzu (*.irs)
Galactic/GRAMS (*.spc, *.fir, *.ir, *.rmn)	JEOL JCAMP (*.wsf)	Thermo/Nicolet (*.spa)
Generic XY Data (*.*)	Mattson (*.ras, *.abs)	

NIR

Sadtler IRF (*.irf)	Generic XY Data (*.*)	Mattson (*.ras, *.abs)
Bomem (*.a01)	GuidedWave (*.*)	PE Spectrum (*.sp)
Bruker (*.*)	Horiba MDW (*.mdw)	Shimadzu (*.irs, *.smf)
Digilab (*.dt)	JASCO (*.jws, *.j1d)	Spectacle/Shimadzu (*.irs)
Galactic/GRAMS (*.spc, *.fir, *.ir, *.rmn)	JCAMP (*.dx, *.jdx)	Thermo/Nicolet (*.spa)

NMR (processed spectra only)

Bruker Aspect (*.*)	JEOL Alice (*.als)	MestRe-C (*.mrc)
Bruker TopSpin (*.1r, *.fid)	JEOL Delta NMR files (*.jdf)	NUTS (*.*)
Bruker UXNMR/XWinNMR 1D (*.1r, *.fid)	JEOL DA-5000 (*.dat)	Sparky NMR (*.ucsf, *.sf)
Bruker UXNMR/XWinNMR 2D (*.2rr)	JEOL GX/GSX/EX-90 NMR files (*.gxd, *.gxp)	Spectacle (*.nmr)
Bruker WinNMR (*.1r, *.fid)	JEOL Mario (*.hed)	Varian 1D NMR (phasefile, data, fid)
Galactic/GRAMS (*.spc, *.fir, *.ir, *.rmn)	JCAMP (*.dx, *.jdx)	Varian 2D NMR (phasefile)
Generic XY Data (*.*)		

MS

Agilent / HP ChemStation (*.d; data.ms)	Generic XY data (*.*)	Mass Evolution EZScan v4 (*.hrd)	Teknivent Vector/2 (*.tkf)
Agilent / HP ChemStation (NT) (*.msd, *.ms)	Hitachi (*.mch)	MassLib JCAMP (*.mlj)	Teknivent Vector/1 (*.raw)
ANDI Mass Spec (*.cdf)	Hitachi M-4100 (ms1.mat)	MatLab (*.mlt)	Teknivent Vector/2 (*.v2s)
Anelva AGS-7000 (*.par)	Hitachi MS Filer (*.msf)	MSS (*.mss)	Text (*.txt)
Anelva AGS-7000 (DOS) (*.par)	HP RTE Chemstation (*.ms)	MS ChemStation (*.ms)	ThermoQuest Xcalibur (*.raw)
Automass (*.spa)	JEOL Compliment (*.hed)	Nermag SIDAR (*.spe)	Varian Saturn (*.ms)
Balzers QuadStar (*.scb)	JEOL DA-5000 (*.dat)	Netsch (*.ntz)	VG 11-250 (*.dat)
EPA (*.ep)	JEOL DA-6000 (*.dat)	netCDF (*.cdf)	VG JCAMP (*.jdx)
Extrel Merlin (*.ms)	JEOL GCMate (*.lrp)	Palisade PAL (*.pal)	VG LabBase (*.hdr)
Finnigan GCQ (*.ms)	JEOL JCAMP (*.jsp)	PE TurboMass (*.raw;_func, *.dat)	VG MassLab (*.raw;_func, *.dat)
Finnigan Incos (*.mi)	JEOL Mario (*.hed)	PE QMass-910 (*.mss)	VG MassLynx (*.raw;_func, *.dat)
Finnigan Ion Trap (*.dat)	JCAMP (*.dx, *.jdx)	Shrader Systems/Windows (*.lrp)	VG MassLynx Processed (*.raw;_func, *.dat)
Finnigan ITS-40 (*.ms)	Kratos DS90 (*.rn)	Shrader System (*.lrp)	VG ThermoLab (*.lgh)
Finnigan Magnum (*.ms)	Kratos Mach3 (*.run)	Shimadzu PAC200 (*.x)	VG ThermoLab (*.ps)
Finnigan SSX (*.dat)	MASPEC (*.mss)	Shimadzu QP-5000 (*.r)	
Galactic/GRAMS (*.spc, *.fir, *.ir)	Mass Evolution (*.spe)		

UV-Vis

Galactic/GRAMS (*.spc, *.fir, *.ir)	JCAMP (*.dx, *.jdx)	PG Instruments (*.spd)	Spectacle (*.uvd)
Generic XY Data (*.*)	JASCO (*.jws)	Shimadzu (*.spc)	

GC

ANDI Chromatography (*.cdf)	Generic XY Data (*.*)
Galactic/GRAMS (*.spc, *.fir, *.ir)	MS ChemStation (*.ms)

Structure File Formats

ChemDraw (*.cdx)	Hampden (*.hsf)	MDL MOL (*.mol)	Smiles structure (*.smi)
ChemWindow (*.cwg)	InChI structure (*.txt)	MDL RXN (*.rxn)	XYZ structure (*.xyz)
DrawIt (*.dsf)	JCAMP (*.dx, *.jdx)		

Data File Formats

MDL SDF (*.sdf)	Infometrix (*.dat)
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KnowItAll Enterprise Solutions Overview

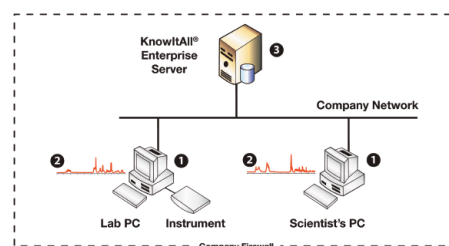
Maximize Productivity: Centralize Access to All Spectra & Chromatograms

Because our primary business is creating spectral databases, we have built our KnowItAll Enterprise Solutions through years of experience in doing just that—building databases. With KnowItAll, your organization can create a data warehouse using these very same technologies. Designated users can then access this data via a secure web browser behind your firewall and ultimately extract more knowledge from these continuously updated, shared resources. **For details visit knowitall.com/enterprise.**

Windows Client

Find Data with SpecFinder™

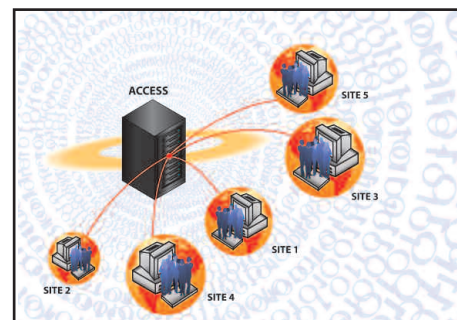
SpecFinder™ is an enterprise-wide tool that continually monitors all computers, servers, instrument systems, and workstations for analytical chemistry data, including spectra, chromatograms, peak tables, and chemical structure files. The data are then indexed and stored on the centralized KnowItAll Enterprise Server.



Server

Store Data with KnowItAll Enterprise Server

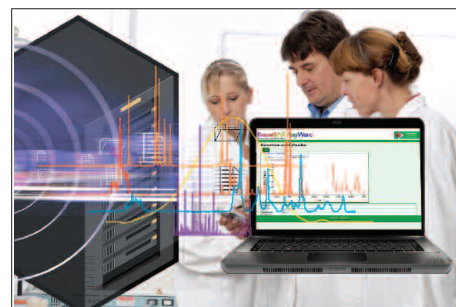
The KnowItAll Enterprise Server is a technology platform designed specifically for the creation of an enterprise-wide Spectral Data Warehouse in a dynamic, heterogeneous laboratory environment. The system is fast, reliable, secure, and scalable, requires minimal support and maintenance, and allows centralized access to all of an organization's spectra, chromatograms, and structures via a single, unified platform.



Web Client

Search Data with KnowItAll AnyWare™

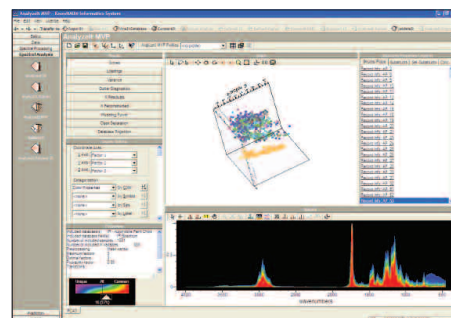
Designated users can access data stored on the KnowItAll Enterprise Server using KnowItAll AnyWare—a powerful browser-based interface designed to search spectra, structures, and related chemical properties securely behind your firewall. No software installation is required, making deployment effortless. It is platform independent and can be used with any web browser, including Internet Explorer, Firefox, Safari, or Chrome.



Windows Client

Analyze Data with KnowItAll Informatics System

Bio-Rad's award-winning KnowItAll Informatics System software for Microsoft Windows allows users to search data stored on the KnowItAll Enterprise Server and offers advanced tools for analyses and reporting so that users can take the data from your warehouse to the next level: knowledge. Tools include: mixture analysis, polymer analysis, overlap density heatmaps, chemometrics, and more. Also includes advanced tools for database building and editing.



Licensing Information

Bio-Rad makes the licensing of their software and databases simple. Individual spectral databases are licensed via USB dongles and software can be licensed via the Internet or USB dongle.

Support & Upgrade Policy

Please visit www.knowitall.com/supportpolicy

Training Options

If you require more training beyond the resources provided (on-line help system, KnowItAll User Manual PDF, demo movies), we would be pleased to discuss additional training options. Please visit www.knowitall.com/training

KnowItAll System Recommendations

Find the latest system recommendations such as operating system, disk space, RAM requirements, and processor at www.knowitall.com/system_recommendations



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