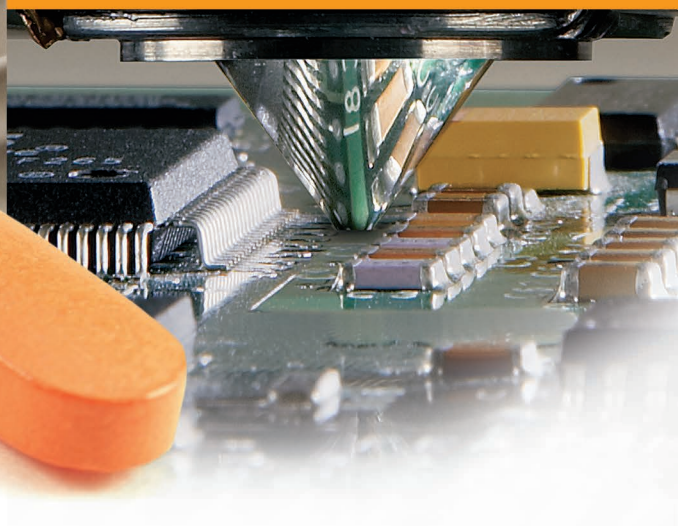
Thermo Scientific
FT-IR and Raman Spectral Libraries



Distinctive spectral libraries

for the most demanding material identification applications

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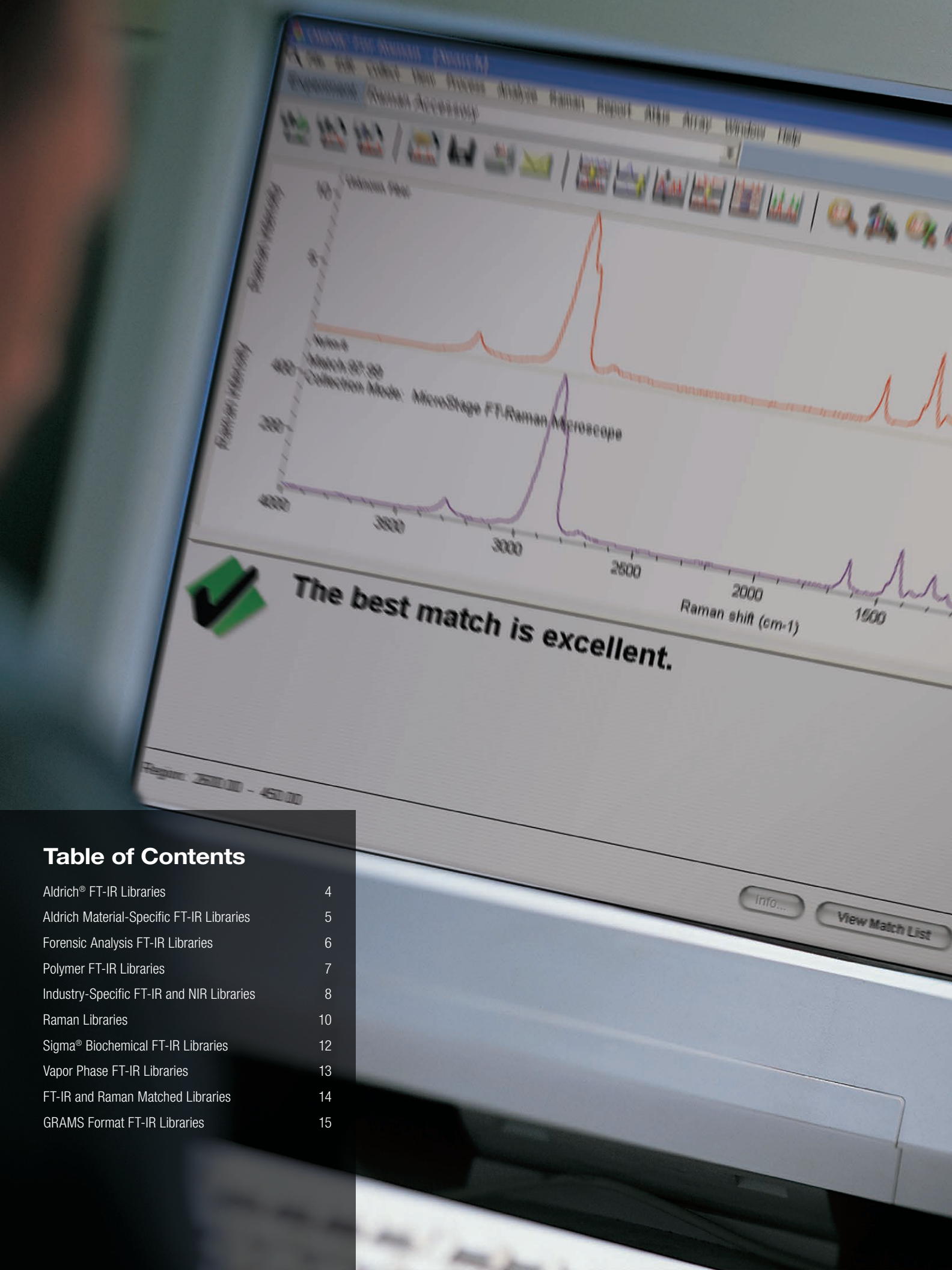

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Thermo Scientific FT-IR and Raman Spectral Libraries

The unique, high quality collections of FT-IR and Raman Spectral Libraries in this catalog are specifically designed to work with Thermo Scientific™ instruments and software. The Thermo Scientific spectral library collection features over 60 databases covering a broad spectrum of mid-IR, near-IR, and Raman data. Spectra are available in condensed or vapor phase, and address a wide range of applications including polymer, pharmaceutical, forensics, and other industry-specific categories.

Unique Collections

We offer a wide variety of FT-IR and Raman spectral library collections, many that are exclusively available for use with Thermo Scientific instruments and software. In fact, we are the only instrument vendor who fully develops, sells and services its own library collections and offers its libraries to users of Thermo Scientific instruments as well as users of instruments from other vendors.

The wide variety of unique, high quality spectral library collections means that you will never have to compromise when choosing libraries for your spectrometer. The data is specifically designed to work with your existing Thermo Scientific system "out-of-the-box"; there is no extra software to buy or install. In addition, we are prepared to assist you when you need new libraries to expand your research, or have questions regarding spectra or searching techniques using any of our collections.

High Quality Data

The quality of the Thermo Scientific high resolution FT-IR and Raman reference collections is exceptional. An exclusive, high spectral resolution and high digital precision format stores the X-axis and Y-axis spectral data in its original, unaltered form. Unlike traditional spectral libraries, this special format produces:

- More accurate search results
- Better data-point accuracy
- Improved quality of spectral matches
- Better spectral subtraction results

For increased flexibility when choosing spectral libraries, we also offer many collections in a traditional, deresolved format that uses less disk space and results in faster searches.

Flexible Configuration

You can choose the configuration of the spectral library data that best meet your laboratory's analytical needs and budget.

- Thermo Scientific™ OMNIC™ or Thermo Scientific™ GRAMS™/ Spectral ID software formats
- High resolution (higher confidence results) or deresolved (faster search speeds) formats
- Large collections such as Aldrich Chemical and Sigma Biochemical are available as full libraries or in libraries of specific chemical entities
- Available on DVD media format

We also offer multiple-copy discounts when you purchase more than one spectral library at a time. For complete details, contact your Thermo Scientific sales representative, or the Thermo Scientific sales office using the information found on the back of this catalog.

Library Formats

We also offer high resolution and deresolved library formats for flexibility in spectral accuracy and search speeds.

See page 5 for an example comparison of high resolution and deresolved spectra.

High Resolution Libraries

High resolution (HR) libraries contain spectra with data points every 2 cm^{-1} (4 cm^{-1} resolution) and have 16-bit Y-ordinate (absorbance scale) precision. Essential for the most accurate spectral subtractions, high resolution spectral libraries are exclusive to Thermo Scientific instruments using OMNIC software.

Deresolved Libraries

Deresolved (DR) libraries contain spectra with data points every 8 cm^{-1} (16 cm^{-1} resolution) and have 8-bit Y-ordinate precision. Deresolved resolution libraries save disk space and speed up searches. They are designed for use with OMNIC, Spectral ID, GRAMS software.

ALDRICH

Aldrich FT-IR Libraries

The Aldrich FT-IR library collections represents a wide variety of the Aldrich Chemical catalog's most common chemicals. The data has been carefully examined and processed by Thermo Fisher Scientific and is available in its entirety, or in material-specific libraries. A comprehensive Aldrich Raman collection is also available. See the Raman Spectral Libraries section for more information.

Aldrich Collection of FT-IR Spectra Edition II (18,454 spectra)

This library represents the most comprehensive collection of FT-IR spectral references available. It contains the most common chemicals found in the *Aldrich Handbook of Fine Chemicals.*

The Aldrich Collection of FT-IR Spectra Edition II library contains spectra of 18,454 pure compounds and comes with the *Second Edition of the Aldrich Library of FT-IR Spectra* (a 3-volume book set). All spectra were acquired by Sigma-Aldrich Co. and were processed by Thermo Fisher Scientific. This library represents the largest collection of spectra collected entirely by FT-IR instrumentation. Eight smaller Aldrich Material Specific Sub-Libraries are also available.

Thermo Scientific™ Nicolet™ Condensed Phase Academic Sampler (1,000 spectra)

This library is suited to the needs of academic institutions and small QC labs. Chosen by chemistry professors from many disciplines, it includes spectra of chemicals used in a wide range of common laboratory experiments.

The Nicolet Condensed Phase Academic Sampler includes 1,000 spectra of common chemicals representing the major functional groups and combinations of functional groups which are most likely to be observed in academic chemistry laboratories. These chemicals are also important building blocks commonly found in industrial applications.

Nicolet Standard Collection of FT-IR Spectra (3,119 spectra)

This collection is suited to the needs of analytical services and investigational laboratories. It provides a wide array of common chemicals in a lower cost package and can be used in combination with the Nicolet Standard Collection of FT-Raman Spectra to provide analysts a higher degree of confidence when identifying unknowns.

The Nicolet Standard Collection of FT-IR Spectra includes 3,119 spectra of common chemicals with representatives of major functional groups and combinations of functional groups. It contains the same chemical series available in the Nicolet Standard Collection of FT-Raman Spectra. These matched libraries can be used alone or in combination with the unique Thermo Scientific OMNIC Linked Search software. (See the FT-IR and Raman Matched library section for more details.)

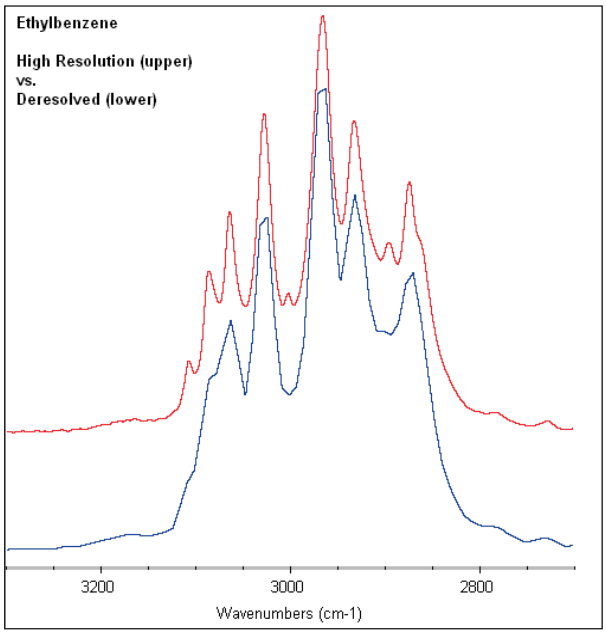
Library	Spectra	Resolution	Part Number
Aldrich Collection of FT-IR Spectra Edition II	18,454	HR	834-016201
Nicolet Condensed Phase Academic Sampler	1,000	HR	834-009800
Nicolet Standard Collection of FT-IR Spectra	3,119	DR	834-004301

HR = High Resolution DR = Deresolved

Aldrich Material-Specific FT-IR Libraries

The Aldrich Material-Specific FT-IR Library collection represents a wide variety of the *Aldrich Handbook of Fine Chemicals* most common chemicals divided by similar functional groups. These spectra were assembled from the Aldrich Collections of FT-IR Spectra Editions I or II, and the data has been carefully examined and processed by Thermo Fisher Scientific.

	Aldrich Edition I – Deresolved Format		Aldrich Edition II – High Resolution Format	
Library	**Spectra Included**	**Part Number**	**Spectra Included**	**Part Number**
Aldrich Alcohols and Phenols	788	834-004701	1,200	834-019600
Aldrich Aldehydes and Ketones	834	834-004801	1,311	834-019700
Aldrich Dyes, Indicators, Alkynes, Nitro and Azo Compounds	753	834-005001	1,229	834-019900
Aldrich Esters, Lactones and Anhydrides	724	834-004901	1,653	834-019800
Aldrich Hydrocarbons	839	834-004601	1,199	834-019500
Aldrich Organometallic, Inorganic, Boron and Deuterium Compounds	632	834-005201	1,523	834-020100
Aldrich Phosphorus and Sulfur Containing Compounds	671	834-005101	822	834-020000
Aldrich Polymers	275	834-005301	466	834-020200
Aldrich Solvents	246	834-008801	246	834-008900



Overlaid spectra of Ethylbenzene from the High Resolution and Deresolved Aldrich Solvents libraries. The upper high resolution spectrum has well-defined peaks that are absent or not as evident in the lower deresolved format. Because of this, the high resolution format will provide better search results.

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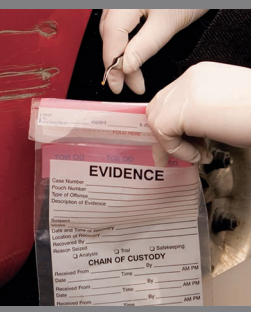

Forensic Analysis FT-IR Libraries

From drugs, to fibers, to weapons of mass destruction, the Thermo Scientific Forensic Analysis FT-IR Libraries cover a wide range of materials of interest to forensic scientists.

Cayman Chemical ATR Designer Drug Library (183 spectra)

The forensic drug library containing spectra of synthetic psychoactive substances based on pure reference material obtained from Cayman Chemicals. The library contains FT-IR spectra of synthetic cannabinoids, synthetic cathinones, synthetic piperazines and tryptamines.

Georgia State Crime Lab Drug (1,940 spectra)

This definitive forensic library is one of the most extensively used collections for the identification of drug substances. The Georgia State Crime Lab Drug Library contains FT-IR spectra of illegal and legal drugs as well as diluents, precursors and other drug-related compounds.

The library consists of 1,940 spectra that were acquired by the Georgia Bureau of Investigation. The samples were secured as pure drug standards from the U.S. Drug Enforcement Administration (DEA), Applied Science Laboratories, U.S. Pharmacopoeial Conventions, Inc., and various pharmaceutical companies. For the majority of samples the material purity is 95% or better and in many cases is greater than 99%. Unless otherwise stated, the samples were prepared for spectral analysis using KBr pellets.

Toronto Forensic (3,549 spectra)

This extensive library is one of the most widely-used collections of its kind for forensic scientists and investigators. The Toronto Forensic Library contains FT-IR spectra of illegal and legal drugs, drug precursors and reagents used to prepare them and other substances encountered in forensic analysis.

The library consists of 3,549 spectra that were measured at the Forensic Laboratories of the Canadian Department of Health and Welfare in Toronto. The spectra are distributed by Thermo Fisher Scientific, under license from Canadian Patent and Development Limited. The spectra are grouped with similar compounds in the library. The major divisions of substances are organic (3,247 spectra), inorganic (183 spectra), and natural and commercial products (127 spectra). For the majority of samples the material purity is 95% or better and in many cases is greater than 99%.

Synthetic Fibers by Microscope (376 spectra)

This library is highly useful for identifying fibers of varying diameters from a wide variety of products and manufacturers. The Synthetic Fibers Library contains FT-IR microscope transmission spectra of synthetic fibers from the Collaborative Testing Services Reference Collection of Synthetic Fibers.

This library consists of 376 spectra that were obtained from a collaborative project between Thermo Fisher Scientific and Dr. Jay A. Siegel and his co-workers in the School of Criminal Justice at Michigan State University. All spectra were measured from pressed samples of the fibers using a Thermo Scientific FT-IR spectrometer and microscope system.

Common Materials and White Powders (469 spectra)

This library is particularly useful to Homeland Security and National Guard investigators. The Common Materials and White Powders Library consists of spectra of commonly found commercial products and white powders.

The library includes 165 spectra of commercially available white powders (e.g., baking soda, flour, Vitamin C) and 304 spectra of other products available on the market. Using this collection, unknown materials can be identified by their commercial names. A more complete identification, which includes chemical information, requires using this collection in combination with other libraries containing solvents, surfactants, polymers, inorganic materials, synthetic fibers, oils and other materials.

The Tennessee Bureau of Investigation (TBI) Gas Phase Library (340 spectra)

The Tennessee Bureau of Investigation (TBI) library includes over 300 spectra collected by the Tennessee Bureau of Investigation Forensics Laboratory on a Thermo Scientific GC-IR system.

The data includes spectra from a wide range of legal and illegal drugs including methcathinones and cannabinoids. The library will be periodically updated with spectra as new drugs appear in criminal cases.

The library is not for sale but may be distributed for free to established and accredited forensics laboratory facilities using Thermo Scientific equipment. Thermo Fisher Scientific is legally bound to state that the library of spectra shall be used only as a tool to determine the identity of a compound, but Thermo Fisher Scientific assumes no responsibility for the use of this data for identification purposes in any legal report or document.

Note: This library can only be ordered by the Customer Special process.

Library	Spectra	Resolution	Part Number
Cayman Chemical ATR Designer Drug Library	183	HR	834-101400
Georgia State Crime Lab Drug	1,940	HR	834-007501
Toronto Forensic	3,549	HR	834-007800
Synthetic Fibers by Microscope	76	DR	834-011100
Common Materials and White Powders	469	HR	834-042200
Tennessee Bureau of Investigation (TBI) Gas Phase Library	340	HR	Special Order–Contact Sales

HR = High Resolution DR = Deresolved

Polymer FT-IR Libraries

The Thermo Scientific Polymer FT-IR Libraries cover a wide variety of polymers and other related end-products, as well as monomers, solvents, and industrial organic chemicals used in polymer production and analysis.

Hummel Polymer and Additives (2,011 spectra)

This library is one of the most comprehensive and commonly used libraries for analysis of polymer materials. It includes spectra of polymers, solvents, monomers and industrial organic compounds and is a valuable resource for anyone involved in the identification of polymers, particularly those working in labs involved in polymer production or analysis.

The Hummel Polymer and Additives Library contains 2,011 spectra collected by Professor Dieter Hummel of the Institute of Physical Chemistry at the University of Cologne (Koln), a recognized specialist in polymer chemistry. This collection was designed to aid analysts in the identification of typical polymer impurities, including excess residual monomers and additives, and indicates the composition of completed products. The library contains additional information such as manufacturer, trade name, literature reference and measurement conditions for each spectrum in the collection.

Polymer Additives and Plasticizers (1,799 spectra)

This library is a valuable addition to any polymer chemist's toolbox. It includes spectra of plastics and additives for polymers, rubbers, cosmetics, adhesives, sealants and plasticizers.

The Polymer Additives and Plasticizers Library features 1,799 spectra collected by Chemir/Polytech Laboratories and Dr. John Kokosa. Each spectrum in the library includes information on manufacturer, chemical name, product name, chemical abstract number, and category name, where available.

Coatings Technology (2,507 spectra)

This library and the included handbook are a highly valuable resource for the analysis of a wide variety of common coating materials. It contains spectra of polymers, resins, vehicles, pigments, extenders, acrylic monomers, radiation-curable monomers, fungicides, mildewcides, inhibitors, stabilizers, solvents and other additives.

The Coatings Technology Library, which is comprised of 2,507 spectra of common coating materials, was prepared by the Federation of Societies for Coatings Technology and includes the revised edition of An Infrared Spectroscopy Atlas for the Coatings Industry (1991). The atlas is the fourth edition of this FSCT publication, dealing with the use of FT-IR in coatings analysis. It includes a 2-volume hardcover book set with valuable reference information on spectroscopy theory, analytical instrumentation, sampling accessories, sample preparation, spectral interpretation and quantitative analysis.

Note: Members of the Federation of Societies for Coatings Technology qualify for a 10% discount when purchasing this library. Please be sure to provide your member number when ordering.

Industrial Coatings (1,961 spectra)

This library is a valuable resource for commercial and industrial laboratories. It includes a wide-range of spectra of monomers, polymers, plasticizers, extenders, solvents, pigments and other additives.

The Industrial Coatings Library consists of 1,961 spectra listed by their trade names.

Rubber Compounding Materials (350 spectra)

This library is a key addition for analyzing materials in the rubber and polymer industries. It contains spectra of accelerators, extenders, plasticizers, as well as curing and other processing aids.

The Rubber Compounding Materials Library includes a total of 350 spectra with descriptive information such as chemical name, manufacturer name and brand name attached to each spectrum.

Library	Spectra	Resolution	Part Number
Hummel Polymer and Additives	2,011	HR	834-008601
Polymers, Polymer Additives and Plasticizers	1,799	HR	834-008300
Coatings Technology	2,507	HR	834-010901
Special Federation of Societies for Coating Technology – Member Pricing		HR	834-010901M
Industrial Coatings	1,961	HR	834-010600
Rubber Compounding Materials	350	HR	834-012000

HR = High Resolution

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Industry-Specific FT-IR and NIR Libraries

The Thermo Scientific Industry-Specific FT-IR and NIR Libraries offer collections of materials commonly found or used in specific industries. These libraries cover typical materials found in a number of manufactured products and manufacturing processes such as solvents, coatings, foods, pulp and paper, lubricants, and pharmaceuticals.

Commercial Materials (212 spectra)

This is a four library set with material-specific collections of commercial interest. It includes spectra of minerals, polypropylene additives, explosives and epoxies.

The Commercial Materials Library contains 212 spectra divided into four material specific segments. The four libraries are:

- Epoxy Resins
  - *48 spectra identified by trade name*
- Explosives
  - *18 spectra (14 explosives, 4 non-explosives) collected by the Georgia State Crime Lab*
- Minerals
  - *56 spectra collected by Professor Paul Painter of Pennsylvania State University*
- Polypropylene Additives
  - *90 spectra of polypropylene additives, solvents and other materials identified by trade name*

Food Additives (519 spectra)

This library features condensed phase FT-IR spectra of compounds of interest to the food industry. The included compounds are on the GRAS (Generally Recognized As Safe) list of US government-approved food additives.

The Food Additives Library features 519 condensed phase FT-IR spectra. These spectra are complementary to the vapor phase spectra included in the Flavors and Fragrances Library (see the Vapor Phase FT-IR Library section.)

Hazardous Chemicals Condensed Phase (411 spectra)

This library contains a collection of condensed phase spectra of toxic chemicals, pollutants and other contaminants. These compounds are of interest to scientists involved in hazardous waste site remediation.

The Hazardous Chemicals Condensed Phase Library has 411 spectra of compounds found on the US Environmental Protection Agency's Office of Toxic Substances consolidated list of chemicals subject to reporting under Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA), also known as the Emergency Planning and Community Right-to-Know Act (EPCRA). This library is complementary to the Hazardous Chemicals Vapor phase Library (see Vapor Phase FT-IR Library section).

Inorganics (1,803 spectra)

This library provides spectra of inorganic and related compounds from around the world. It consists of minerals, boron compounds, general inorganic substances and inorganic materials of commercial interest.

The Inorganics Library contains a total of 1,803 spectra, including 600 minerals, 296 boron compounds, 698 other inorganic substances and 211 commercial materials. The commercial materials include cements, ceramics, porcelain, clay, glass and other raw materials.

Lubricants and Oils (1,576 spectra)

This library consists of spectra representing an international collection of lubricants and oils. It includes spectra of motor oils, gear oils, electro insulating oils, machinery oils, turbine oils, compressor oils, hydraulic oils, anticorrosion oils, steam cylinder oils, metal-cutting oils, natural oils, silicone oils, fuels, greases, and solvents.

The Lubricants and Oils Library is an international collection of 1,576 spectra of motor oils, electro insulating oils, machinery oils, turbine oils, compressor oils, hydraulic oils, anticorrosion oils, steam cylinder oils, metal-cutting oils, mineral oils, synthetic oils, biologically-derived oils, silicone oils, fuels, greases and solvents. It contains a transmission library of over 1000 spectra collected by KBr liquid cell. Additionally, it contains ATR libraries of over 500 spectra in both ATR-corrected and uncorrected formats. A detailed User's Guide is included, which provides an overview of lubricant analysis, a description of the sampling techniques used, a list of the most common oil additives, and a table of typical compounds used in synthetic oils and additives and their associated FT-IR absorption bands.

Minerals (600 spectra)

This library is a subset of the Inorganics Library. It contains minerals from all over the world.

The Minerals Library contains the spectra of 600 minerals and includes information on the mineralogical name, chemical formulas, occurrence and color.

Near-IR Pharmaceutical Reference Database (385 spectra)

This library offers an FT-NIR spectral library collection of active and inactive pharmaceutical substances. It can be used to: identify unknown samples, as a reference when setting up qualitative NIR methods or as a comparison against known sample spectra.

The Near-IR Pharmaceutical Reference Database is a collection of 385 pharmaceutical compounds including both active and inactive substances. Solid samples were collected in reflectance using a Thermo Scientific™ SabIR™ fiber optics probe. Liquid samples were collected in transmittance using a 2 mm quartz cell.

Nicolet Condensed Phase Sampler (842 spectra)

This unique collection of infrared spectra from multiple libraries is designed to cover a wide range of investigative needs. It is designed to facilitate high productivity in a cost-effective package for investigative laboratories.

The Nicolet Condensed Phase Sampler Library is a compilation of 842 spectra of drugs, polymers, inorganics, and general chemicals that can be used for investigation of unknown samples.

Paper Materials (302 spectra)

This library provides direct access to spectra of materials used in the production of paper products. The spectra were chosen to aid in the identification of impurities as well as to indicate the composition of completed paper products.

The Paper Materials Library includes 302 spectra of compounds and materials used in the production of paper products. The spectra were collected using a variety of techniques, including transmission and ATR.

Pharmaceutical Excipients (300 spectra)

This library is designed for those laboratories studying pharmaceutical formulations using FT-IR spectroscopy. It provides high quality FT-IR spectra of the most common pharmaceutical excipients.

The 300 spectra in the Pharmaceutical Excipients Library were collected using a Thermo Scientific FT-IR spectrometer. All materials were tested via current United States Pharmacopoeia compendium methodology for identity and purity – only materials that passed these methods were used to create this library. Customers may purchase the library as an FT-IR only, Raman only (see Raman Library section) or as a matched FT-IR and Raman library (see FT-IR and Raman Matched Library section). It includes a textbook explaining spectroscopy techniques and the spectra of pharmaceutical excipients for reference use.

Pharmaceutical Excipients Library was created in collaboration with David E. Bugay and W. Paul Findlay of Bristol-Myers Squibb Pharmaceutical Research Institute. The spectra were collected using a Nicolet FT-IR spectrometer from Thermo Scientific. All solid phase excipients were sampled for FT-IR analysis using diffuse reflectance to assure that the spectra truly represented the physical nature of the pharmaceutical solid.

Surfactants (637 spectra)

This library provides a comprehensive collection of surfactant spectra. It is designed for use by scientists with an interest in surfactants and related materials.

The Surfactants Library consists of 637 carefully characterized surfactant spectra organized by trade name and formula. They were run and compiled by Clara Craver of Chemir Analytical Services.

US Geological Survey Minerals (78 spectra)

This library features spectra of carefully characterized minerals. It represents a group of naturally occurring minerals of interest in geological investigations.

The US Geological Survey Minerals Library includes 78 spectra of carefully characterized minerals collected by the US Geological Survey. Most samples were from the Smithsonian National Museum of Natural History. The rest were from the Hunt and Salisbury collection in Denver and a variety of other sources. Most of the minerals represented in the library are silicates. It includes four spectral reference files of each mineral:

1. Reflectance spectrum of a 0–74 micron particle size sample
2. Reflectance spectrum of a 74–250 micron particle size sample
3. Reflectance spectrum of a solid sample
4. Transmittance spectrum

Library	Spectra	Resolution	Part Number
Commercial Materials	213	DR	834-010101
Food Additives	519	HR	834-010300
Hazardous Chemicals Condensed Phase	411	HR	834-011401
Inorganics	1,803	HR	834-025800
Lubricants and Oils	1,576	HR	834-016000
Minerals	600	HR	834-025700
Near-IR Pharmaceutical Reference Database	385	HR	834-024301
Nicolet Condensed Phase Sampler	842	HR	834-018300
Paper Materials	300	HR	834-013900
Pharmaceutical Excipients	300	HR	834-019201
Surfactants	637	HR	834-009100
US Geological Survey Minerals	78	DR	834-009600

HR = High Resolution DR = Deresolved

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Raman Libraries

Raman spectra are ideal for library searching because they are comprised of relatively sharp, distinct bands with very little interference from water, highly polar bonds and additives such as Nujol. The Thermo Scientific Raman Libraries cover a number of key chemical categories and should be part of any analyst's toolbox for performing material identification. Our Raman Libraries offer analysts the same advantages available with the Thermo Scientific FT-IR databases and are valuable for those using dispersive and FT-Raman. FT-IR and Raman spectroscopies are complementary techniques, each looking at a different aspect of a sample's molecular composition.

Law Enforcement and Security (LEnS) Raman Library (8,550 spectra)

This library includes spectra of specific interest to the law enforcement and security communities. The library includes a wide variety of compounds and solutions spanning narcotics and other pharmaceuticals, household and industrial chemicals, pesticides, energetics, and laboratory reagents. It also features chemicals identified by the International Task Force (ITF) and National Institutes of Occupational Safety and Health (NIOSH) as being specifically hazardous and/or posing occupational hazards. The data was collected on a dispersive Raman system using NIR excitation, and has been corrected for instrument response (white light corrected).

Aldrich Raman Condensed Phase (14,033 spectra)

This library represents the most comprehensive collection of FT-Raman spectral references available. It contains many common chemicals found in the *Aldrich Handbook of Fine Chemicals.*

To create the Aldrich Raman Condensed Phase Library, 14,033 compounds found in the Aldrich Collection of FT-IR Spectra Edition II Library were excited with an Nd:YVO4 laser (1064 nm) using laser powers between 400–600 mW, measured at the sample. A Thermo Scientific FT-Raman spectrometer (with a Ge detector) was used to collect the Raman spectra. The spectra were saved in Raman Shift format.

Nicolet Standard Collection of Raman Spectra (3,119 spectra)

This collection is suited to the needs of analytical services and investigational laboratories. It provides a wide array of common chemicals in a lower cost package that can be used in combination with the Nicolet Standard Collection of FT-IR Spectra to provide analysts a higher degree of confidence when identifying unknowns.

The Nicolet Standard Collection of Raman Spectra includes 3,119 spectra of common chemicals with representatives of major functional groups and combinations of functional groups. It contains the same chemical series available in the Nicolet Standard Collection of FT-IR Spectra. These matched libraries can be used alone or in combination with our unique OMNIC Linked Search software. (See the FT-IR and Raman Matched Library section for more details.)

Raman Forensics (175 spectra)

This library is designed to assist forensic scientists and investigators. It contains a collection of common drug and related compounds that are frequently encountered in the course of forensic analysis.

The Raman Forensic Library is a collection of 175 drug compounds, excipients, precursors, and metabolites. The Raman technique provides a unique benefit in forensic science since sample analysis can be completed directly through plastic bags and containers.

Raman Organic Chemical Collection (1,000 spectra)

This library contains a wide selection of organic chemicals. It provides chemists with a broad range of functional groups to aid chemical investigations.

The Nicolet Raman Organic Chemical Library provides 1000 organic chemical spectra. All samples were run by us using the Thermo Scientific FT-Raman spectrometer.

Raman Pharmaceutical Excipients (300 spectra)

This library is designed for those laboratories studying pharmaceutical formulations using Raman spectroscopy. It provides high quality Raman spectra of the most common pharmaceutical excipients.

The 300 Raman spectra in the Pharmaceutical Excipient Library were collected using an FT-Raman spectrometer. All materials were tested via current United States Pharmacopoeia compendium methodology for identity and purity – only materials that passed these methods were used to create this library. Customers may purchase the library as Raman only or as a matched FT-IR and Raman library (see FT-IR and Raman Matched Library section), or may purchase an FT-IR only library (see Industry-Specific FT-IR and NIR Library section). It includes a textbook with explanation of spectroscopy techniques and the spectra of the pharmaceutical excipients.

The Pharmaceutical Excipients Library was created in collaboration with David E. Bugay and W. Paul Findlay of Bristol-Myers Squibb Pharmaceutical Research Institute. The spectra were collected using a Thermo Scientific FT-Raman spectrometer.

Raman Polymer (99 spectra)

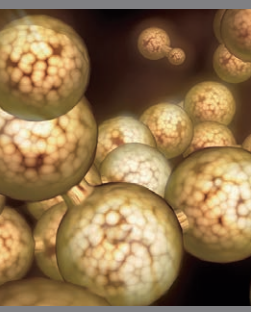
This is a convenient library which provides an introduction to the Raman analytical technique for polymer analysis. The polymer reference samples were prepared by scientific polymer products.

The Raman Polymer Library includes 99 spectra of industrially important polymers.

Library	Spectra	Resolution	Part Number
Law Enforcement and Security (LEnS) Raman	8550	HR	834-091200
Aldrich Raman Condensed Phase	14,033	HR	834-004001
Nicolet Standard Collection of Raman Spectra	3,119	DR	834-004101
Raman Forensics	175	HR	834-014201
Raman Organic Chemical Collection	1,000	DR	834-004401
Raman Pharmaceutical Excipients	300	HR	834-019301
Raman Polymer	99	HR	834-014101

HR = High Resolution *DR = Deresolved*

Sigma Biochemical FT-IR Libraries



The Thermo Scientific Sigma Biochemical FT-IR Libraries contain chemicals found in the Sigma Chemical Catalog of particular interest to those engaged in biochemical research or QC applications. The data was collected Sigma-Aldrich Chemical Corporation, carefully examined and processed by Thermo Fisher Scientific and is available in its entirety or in chemical subset collections.

Sigma Biochemical Condensed Phase (10,411 spectra)

This library provides a comprehensive spectral collection of the most common chemicals found in the *Sigma Biochemicals and Regents* catalog. It includes an extensive combination of spectra of interest to the biochemical field.

The Sigma Biochemical Condensed Phase Library contains 10,411 spectra acquired by Sigma-Aldrich Co. which were examined and processed at Thermo Fisher Scientific. These spectra represent a wide range of chemical classes of particular interest to those engaged in biochemical research or QC.

Sigma Steroids (3,011 spectra)

This library includes a wide variety of natural and synthetic steroids. It provides high-quality spectral data for medical and biochemical research and QC.

The Sigma Steroids Library contains 3,011 spectra. The steroid spectra were acquired by Sigma and the United Kingdom Medical Research Council. Spectra are ordered within the library by skeletal type, and further by degree and type of substitution and unsaturation.

Material-Specific Libraries

Five material-specific libraries covering related chemical classes of the Sigma Biochemical Condensed Phase Library are available. They allow investigators to focus on specific compounds of interest to them.

These material-specific libraries are subsets of the Sigma Biochemical Condensed Phase Library and include:

- Dyes, Stains and Natural Pigments
- Enzymes, Coenzymes and Enzyme Substrates
- Fatty Acids, Glycerides, Oils and Waxes
- Proteins and Peptides
- Sugars and Carbohydrates

Library	Spectra	Resolution	Part Number
Sigma Biochemical Condensed Phase	10,411	HR	834-005501
Sigma Steroids	3,011	HR	834-008101
Sigma Dyes, Stains and Natural Pigments	628	DR	834-006001
Sigma Enzymes, Coenzymes and Enzyme Substrates	485	DR	834-005801
Sigma Fatty Acids, Glycerides, Oils and Waxes	766	DR	834-006101
Sigma Proteins and Peptides	747	DR	834-005701
Sigma Sugars and Carbohydrates	614	DR	834-005901

HR = High Resolution DR = Deresolved

Vapor Phase FT-IR Libraries

Thermo Scientific has an extensive collection of Vapor Phase FT-IR Libraries cover a wide range of materials, from hazardous chemicals to flavors and fragrances. They are used extensively in infrared analysis using hyphenated techniques including GC-IR and TGA-IR for identification of unknown constituents.

Aldrich Vapor Phase (6,611 spectra)

This library is an ideal tool for investigator using FT-IR to analyze gas phase materials. It contains gas phase spectra collected by Aldrich using a GC-IR interface to ensure chromatographically pure samples.

The Aldrich FT-IR Vapor Phase Library contains 6,611 gas phase FT-IR spectra collected by Aldrich Chemical Company using a GC interface. The GC interface reduces the sample decomposition common when vapor phase spectra are obtained in a conventional gas cell. 5,010 spectra are included in the Aldrich Vapor Phase Library.

EPA Vapor Phase (3,300 spectra)

This library provides a focused collection of gas phase spectra of interest in environmental monitoring. It contains materials selected for inclusion by the US Environmental Protection Agency (EPA).

The EPA Vapor Phase Library was acquired by the Environmental Protection Agency (EPA) in the late 1970s and early 1980s. The collection of 3,300 gas phase spectra was collected with a heated gas cell for use in the identification of typical GC-IR eluents.

Flavors and Fragrances (667 spectra)

This library is a collection of vapor phase chemical compounds of interest to food and cosmetic scientists. It contains a wide array of spectra of chemicals which contribute fragrance and flavor to commercial products.

The Flavors and Fragrances Library includes 667 vapor phase spectra of materials with flavor or fragrance properties. Most of the spectra were collected by Aldrich using a GC interface to reduce contamination and decomposition. All spectra are on the GRAS (Generally Recognized as Safe) list of US government-approved foods. These spectra are complementary to the condensed phase spectra included in the Food Additives Library (see the Industry-Specific FT-IR and NIR Library section).

Hazardous Chemicals Vapor Phase (304 spectra)

This library contains vapor phase spectra of toxic chemicals, pollutants and other contaminants. It is a collection of specific hazardous materials found on the EPA's Toxic Chemical list.

The Hazardous Chemicals Vapor Phase Library contains 304 spectra which are on the US Environmental Protection Agency's Office of Toxic Substances consolidated list of chemicals subject to reporting under Title III of the Superfund Amendments and Reauthorization Act of 1986, a.k.a., the Emergency Planning and Community Right-to-Know Act. This library is complementary to the Hazardous Chemicals Condensed Phase Library (see Industry-Specific FT-IR and NIR Library section).

Nicolet FT-IR Vapor Phase (8,654 spectra)

This library is one the most comprehensive collections of vapor phase FT-IR spectra. It is an invaluable tool for scientist involved in investigations on gas phase materials.

The Vapor Phase Library contains 8,654 FT-IR spectra of compounds measured in gas phase. Most spectra were acquired by the Sigma-Aldrich Co. using product samples. Additional spectra were collected by application scientists from Hannover University, University of Wurzburg and Thermo Fisher Scientific.

TGA Vapor Phase (460 spectra)

This library includes spectra of compounds likely to evolve during TGA/FT-IR experiments. It is an extremely valuable tool for chemists studying composition and decomposition material properties.

The TGA Vapor Phase Library contains 460 spectra FT-IR of compounds commonly found when running TGA/FT-IR studies. It identifies most low molecular weight gases. Investigators searching for spectra of more exotic species or for more combinations of functional groups should consider the Nicolet FT-IR Vapor Phase Library.

Library	Spectra	Resolution	Part Number
Aldrich Vapor Phase	6,611	HR	834-006300
EPA Vapor Phase	3,300	HR	834-006900
Flavors and Fragrances	667	HR	834-009400
Hazardous Chemicals Vapor Phase	304	HR	834-011700
Nicolet FT-IR Vapor Phase	8,654	HR	834-006600
TGA Vapor Phase	460	HR	834-007200

HR = High Resolution

Thermo SCIENTIFIC

FT-IR and Raman Matched Libraries

Available only for use with our OMNIC spectroscopy software, the Thermo Scientific FT-IR and Raman Matched Libraries offer researchers and analysts a unique tool in performing material identification. Using these libraries with the OMNIC Linked Search software compares both an FT-IR and Raman spectrum of the sample against a matched set spectral reference data in the libraries. Matching the sample via types of spectra and collating the results greatly increases the quality of search which increases the confidence in the results for making a positive identification OMNIC Linked Search software is required, and is included with the Matched Libraries. It also can be purchased separately for customers who already own the individual libraries.

Nicolet Standard Collection of FT-IR and Raman Matched Spectra (3,119 FT-IR and 3,119 Raman spectra)

This library is ideal for those laboratories that have both FT-IR and Raman spectra available. It contains a wide array of common chemicals found in the *Aldrich Handbook of Fine Chemicals.*

The Nicolet Standard Collection of Matched and Raman Spectra provides 3,119 FT-IR spectra and 3,119 Raman spectra that are of general interest to the analytical laboratory customer. This library contains a subset of the Aldrich FT-IR Condensed Phase Library along with matching Raman spectra of the same compounds. Combined searching requires OMNIC Linked Search software which is included with the package.

Pharmaceutical Excipients Matched FT-IR and Raman (300 FT-IR and 300 Raman spectra)

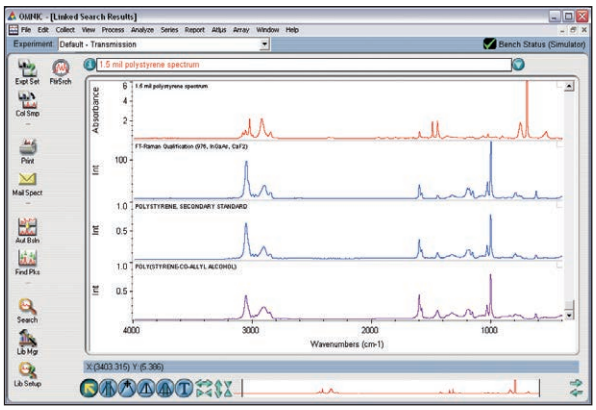
This collection is designed for those laboratories studying pharmaceutical formulations using FT-IR and Raman. It provides high quality FT-IR and Raman spectra of common pharmaceutical excipients.

This spectral collection contains 300 matched FT-IR and Raman spectra collected using Thermo Scientific FT-IR and FT-Raman spectrometers. All materials were tested via current United States Pharmacopoeia compendium methodology for identity and purity – only materials that passed these methods were used to create this library. Customers may purchase the library as FT-IR only (see Industry-Specific FT-IR and NIR Libraries), Raman only (see Raman Spectral Libraries section) or a matched FT-IR and Raman library. It includes a textbook with explanation of spectroscopy techniques and the spectra of pharmaceutical excipients for reference use. Combined searching requires the OMNIC Linked Search software, which is included with the package.

The Pharmaceutical Excipients Matched FT-IR and Raman Library was created in collaboration with David E. Bugay and W. Paul Findlay of Bristol-Myers Squibb Pharmaceutical Research Institute. The spectra were collected using Thermo Scientific FT-IR and FT-Raman spectrometers.

Library	Spectra	Resolution	Part Number
Nicolet Standard Collection of FT-IR and Raman Matched Spectra	3,119 FT-IR/3,119 Raman	DR	833-009601
Pharmaceutical Excipients Matched FT-IR and Raman	300 FT-IR/300 Raman	HR	834-020301
OMNIC Linked Search Software	N/A	N/A	834-004200

HR = High Resolution DR = Deresolved



Search results for polystyrene sample in the exclusive OMNIC Linked Search software

GRAMS Format FT-IR Libraries

The following libraries are available for use with GRAMS and Spectral ID software. They are only available in deresolved format.

Library	Spectra	Resolution	Part Number
Aldrich Collection of FTIR Spectra Edition II	18,454	DR	835-006000
Aldrich Raman Condensed Phase	14,033	DR	835-005100
Aldrich Vapor Phase	6,611	DR	829-035400
Coatings Technology	2,507	DR	829-125400
Coatings Technology Member Price	2,507	DR	829-125400M
Condensed Phase Academic Sampler	1,000	DR	829-195400
Hummel Polymer and Additives	2,011	DR	829-045400
Flavors and Fragrances	667	DR	829-105400
Hazardous Chemicals Vapor Phase	304	DR	829-235400
Polymer Additives and Plasticizers	1,799	DR	829-275400
Rubber Compounding Materials Condensed Phase	350	DR	829-225400
Synthetic Fibers Library	76	DR	829-095400

DR = Deresolved

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Switzerland +41 61 716 77 00
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