ThermoFisher
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NIST Trace Evidence Workshop
Advancing Technology and Measurement in Forensic Science

Thermo Fisher Databases for Forensics

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FT-IR and Raman Databases / Libraries Overview

Thermo Scientific FT-IR and Raman Spectral Databases

- Offer unique, high quality collections of FT-IR and Raman Spectral Libraries encompassing some 258,000 compounds.
- The Thermo Scientific – Nicolet spectral library collection features over 60 databases covering a broad spectrum of Mid-IR, Near-IR, and Raman databases.
- IR Databases or Libraries created using accessories for ATR – Attenuated Total Reflection AND Transmission via Films, Mulls, Liquid cells and Pellets
- Qualitative Spectra Databases are available in **condensed or vapor phase**, and address a wide range of applications relevant to Forensics Labs with Chemical, Polymer, Pharmaceutical, Forensics, Biochemical and other industry-specific categories.
  - Quantitative Spectra are available in **vapor phase** Gas Method Calibrations utilized for multi-component gas analysis in investigative research. Fire Science, ABO (DOD), etc.
- Software products to identify unknowns and for multi-component identification.

Commercial FT-IR and Raman Spectral Libraries / Databases

- **Two Library Formats**
  - high resolution and deresolved library formats for flexibility in spectral accuracy and search speeds.
- **High Resolution Libraries**
  - High resolution (HR) libraries contain spectra with 2 cm-1 resolution and have 16-bit Y-ordinate (absorbance scale) precision...
- • More accurate search results
- • Better data-point accuracy
- • Improved quality of spectral matches
- • Better spectral subtraction results
- **Deresolved Libraries**
  - Deresolved (DR) libraries contain spectra with 8 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 various OMNIC, Specta ID, GRAMS, etc. software.

Thermo Nicolet HR Database Collection Parameters

- FT-IR Databases created at Thermo R&D - Manufacturing in Madison, WI, USA and with various Government or Industrial customer partnerships / assistance.

- **Gas / Vapor Phase** –
- Qualitative AND Quantitative Databases
- 4,000 to 400 cm-1 spectral range
- 0.5 cm-1 Spectral Resolution
- 256 scans (5 min) Background and Sample
- Happ-Genzel apodization for consistency

- **Quantitative Method Calibration Databases** consist of hundreds of compounds spectra run at various concentrations for precision and accuracy.

- **Mid-IR** –
- 4,000 to 400 cm-1 spectral range
- 2 cm-1 Spectral Resolution
- 256 scans (5 min) Background and Sample
- Happ-Genzel apodization for consistency
- **Near-IR -**
- 10,000 to 4,000 cm-1 spectral range
- Same as Mid-IR above

- **Raman** – FT and Dispersive created
- 4,000 to 50 cm-1 spectral range
- 2 cm-1 Spectral Resolution
- FT - 256 scans (`5 min) Background and Sample OR
- Dispersive -5 sec to 5 min sample collection

Chemical Databases / Libraries

- **ALDRICH COLLECTION FT-IR SPECTRA EDITION II** This library represents the most comprehensive collection of FT-IR spectral references available. It contains the most common chemicals collection of: hydrocarbons, alcohols, phenols, aldehydes, ketones, esters, anhydrides, lactones, dyes, indicators, alkynes, nitro and azo compounds, phosphorous, sulphur containing compounds, inorganics & silanes
- **ALDRICH RAMAN CONDENSED PHASE LIBRARY** Library consists of comprehensive Raman spectra of various substances, most of which are pure organic or inorganic compounds. To create this library, the compounds in the Aldrich FT-IR Condensed Phase library were excited with an Nd:YVO4 laser (1064 nm) using laser powers between 400 - 600mW, measured at the sample. A Thermo Scientific Raman spectrometer (with a Ge detector) was used to collect the Raman spectra. The spectra were then saved in Raman Shift format. All of the spectra were originally measured at a resolution of 2 cm-1.

SIGMA BIOCHEMICAL LIBRARY A collection of over 10,000 of the most common chemicals found in the Sigma Chemical catalog. These spectra were acquired by Sigma and examined and processed at Thermo Fisher Scientific and represent a wide range of functional groups of particular interest to those engaged in biochemical research or QC. Sigma Proteins and Peptides Library Sigma Enzymes, Coenzymes and Enzyme Substrates Library Sigma Sugars and Carbohydrates Library Sigma Dyes, Stains and Natural Pigments Library Sigma Fatty Acids, Glycerides, Oils and Waxes Library

SIGMA STEROIDS LIBRARY A collection of over 3000 spectra of steroids available from Sigma or provided to Sigma by the UK Medical Research Council.

HAZARDOUS CHEMICALS CONDENSED PHASE LIBRARY A collection of toxic chemicals, pollutants and other contaminants of interest.

Forensic Databases / Libraries

- **CAYMAN CHEMICAL ATR DESIGNER DRUG LIBRARY** Forensic drug library spectra of synthetic psychoactive substances based on pure reference material of synthetic cannabonoids , synthetic cathinones, synthetic piperazines and tryptamines.
- **GEORGIA STATE CRIME DRUG LIBRARY** A collection of illicit and licit drugs acquired in the condensed phase by the Georgia Bureau of Investigation
- **TORONTO FORENSIC LIBRARY** A collection of illicit and licit drugs in various morphologies, physical states, and salt forms, as well as drug precursors, diluents and contaminants. It is supplemented by chemical reagents and spectra of other substances encountered as physical evidence.
- **SYNTHETIC FIBERS LIBRARY** Of interest to forensic labs and others who do fibers work. Samples were acquired from the National Bureau of Standards, and were run on a microscope
- **TENNESSEE BUREAU OF INVESTIGATION (TBI) GAS PHASE LIBRARY** Library includes spectra collected by TBI Forensics Laboratory on a Thermo Nicolet GC-IR system. The data includes spectra from a wide range of legal and illegal drugs including methcathinones and cannabinoids.
- **COMMON MATERIALS AND WHITE POWDERS LIBRARY** Library combination includes spectra of commercially available white powders (baking soda, flour, Vitamin C) spectra of other products available on the market. Unknown materials can be identified by their commercial names.
- **THERMO LAW ENFORCEMENT and SECURITY (LEnS) Raman Library** narcotics and other pharmaceuticals, household and industrial chemicals, pesticides, laboratory reagents, explosives, energetic materials and chemical warfare agents ~ 8,550 unique precursors, compounds and breakdown product spectra **Note:** Also FT-IR Library Version.
- **COMPREHENSIVE FT-IR FORENSIC (**4,286) PAINTS, controlled substances, drugs, explosives, energetic materials & other materials

Industrial Databases / Libraries

- **SURFACTANTS LIBRARY -** A comprehensive collection of carefully characterized surfactant spectra organized by trade name and formula.

LUBRICANTS AND OILS LIBRARY This is an international collection of spectra of motor oils, gear oils, electroinsulating oils, machinery oils, turbine oils, compressor oils, hydraulic oils, anticorrosion oils, steam cylinder oils , metal-cutting oils, natural oils, silicone oils, fuels, greases, solvents and most common motor oil additives.

FOOD ADDITIVES LIBRARY A collection of spectra of compounds of interest to the food industry selected from the Aldrich and Sigma libraries.

PHARMACEUTICAL EXCIPIENTS LIBRARY This spectral library contains 300 matched IR and Raman spectra collected using Thermo Scientific FT-IR and FT-Raman spectrometers.

NEAR INFRARED PHARMACEUTICAL REFERENCE DATABASE A reference database for near infrared users containing pharmaceutical compounds of both active and inactive substances.

PAPER MATERIALS LIBRARY The Paper Materials Library includes compounds and materials used in the production of paper products. aid in the identification of impurities and to indicate the composition of completed paper products.

INORGANICS LIBRARY The Inorganics library contains four basic subgroups: Minerals (600 spectra), Borons (296 spectra), Inorganic Compounds (698 spectra) and Commercial Materials (211 spectra).

US GEOLOGICAL SURVEY MINERAL LIBRARY A collection of carefully characterized minerals acquired by the USGS.

Vapor Phase Databases / Libraries

- **NICOLET VAPOR PHASE LIBRARY** All the spectra from the Aldrich Vapor Phase Library augmented with spectra from Hannover University, University of Wurzburg and Thermo Scientific's applications scientists to total 8,654 spectra.
- **TGA VAPOR PHASE LIBRARY** This collection contains 460 spectra of compounds most likely to evolve during heating, drawn from the Nicolet Vapor Phase Library.
- **EPA VAPOR PHASE LIBRARY** This is a collection of 3,300 spectra acquired by the EPA in the late 1970's and early 1980's. The spectra were not run on a GC/FT-IR.
- **HAZARDOUS CHEMICALS VAPOR PHASE LIBRARY** A collection of 304 vapor phase spectra of toxic chemicals, pollutants and other contaminants of interest.
- **FLAVORS AND FRAGRANCES LIBRARY** A collection of vapor phase spectra of compounds of interest to the flavors and fragrance industry selected from the Aldrich and Sigma libraries.

Things to Consider When Collecting Sample Spectra

- Spectral Quality
  - Measurement time
  - Apodization
- Resolution and data point spacing
  - Higher resolution may provide more differentiation.
  - Higher resolution = more noise
  - Longer collection time
- Scaling and weighting intensity
  - Scale largest peak to one
  - Scale on importance or data quality (fingerprint region from about 1500 to 500 cm^{-1} usually contains a series of absorptions)
- Spectral Processing
  - Baseline Correction: Minimum to zero
  - Main Solvent/Component Suppression
  - Advanced ATR Correction
  - Derivative or smoothing

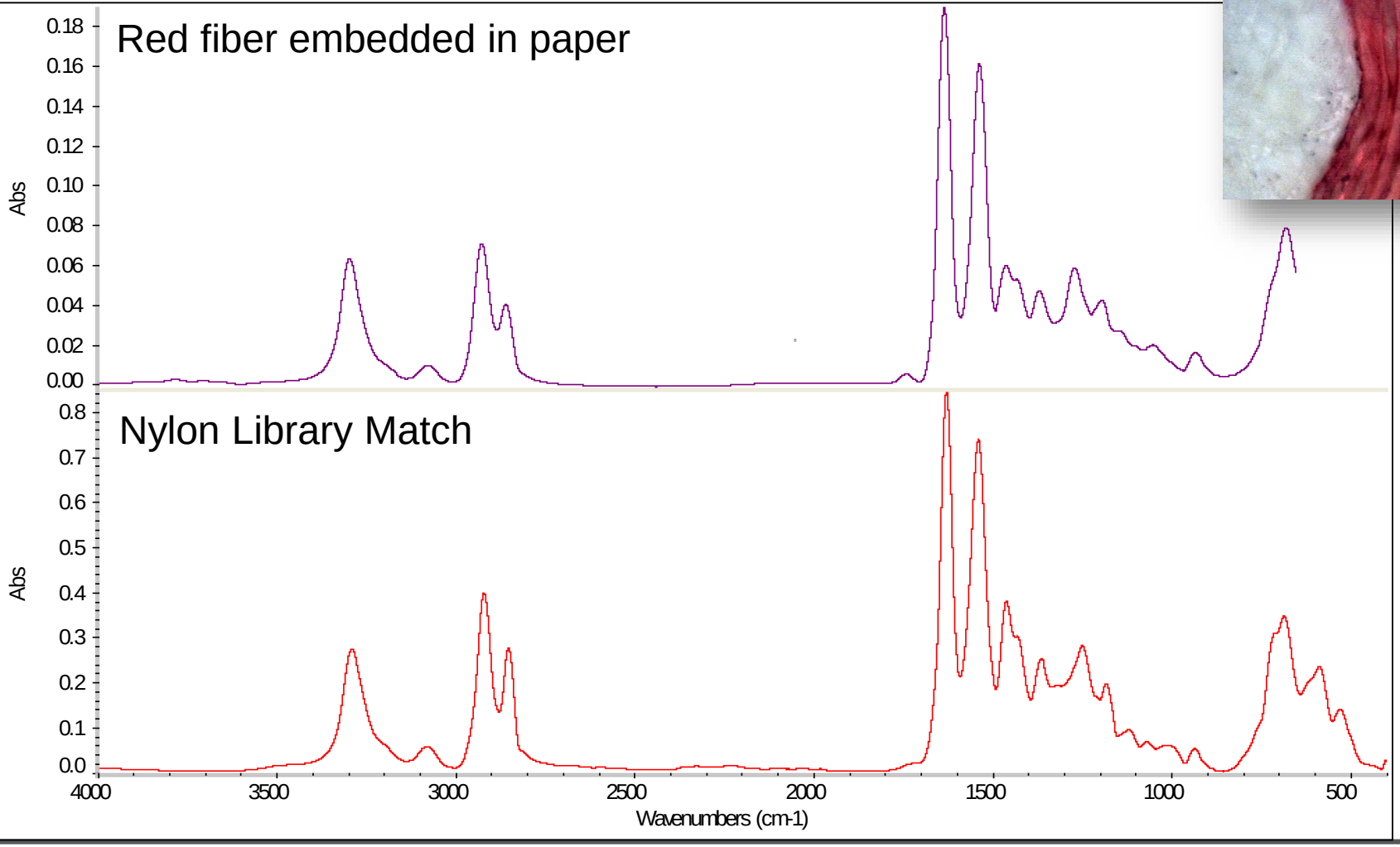
Things to Consider When Collecting Spectra
Select a spectral range that is appropriate to your application

- Most infrared peaks occur between 4000 cm-1 and the low end cutoff based on the accessory as well as the detector and beamsplitter. Most instruments have a Mid-IR KBr beamsplitter and DTGS detector that provide a low end around 400 cm-1.
- Far-IR 700 to 10 cm-1 can extend the low end for inorganic identification and organic overtones.
- Near-IR 12800 to 2800 cm-1 - Most organic compounds have combination bands above 4000 cm-1 that might provide some useful information.
- Raman spectra databases cover broad 4000 to 50 cm-1 spectral range.
- Libraries save the spectra as absorbance.

Material ID Library Search
Single Compound Identification

Embedded Fibers - ATR

- Omnic Library Search – set number Library hits 1 to 10
- Quick analysis of security threads and embedded fibers
- Library Match, Subtract, Lib Match 2nd component, etc



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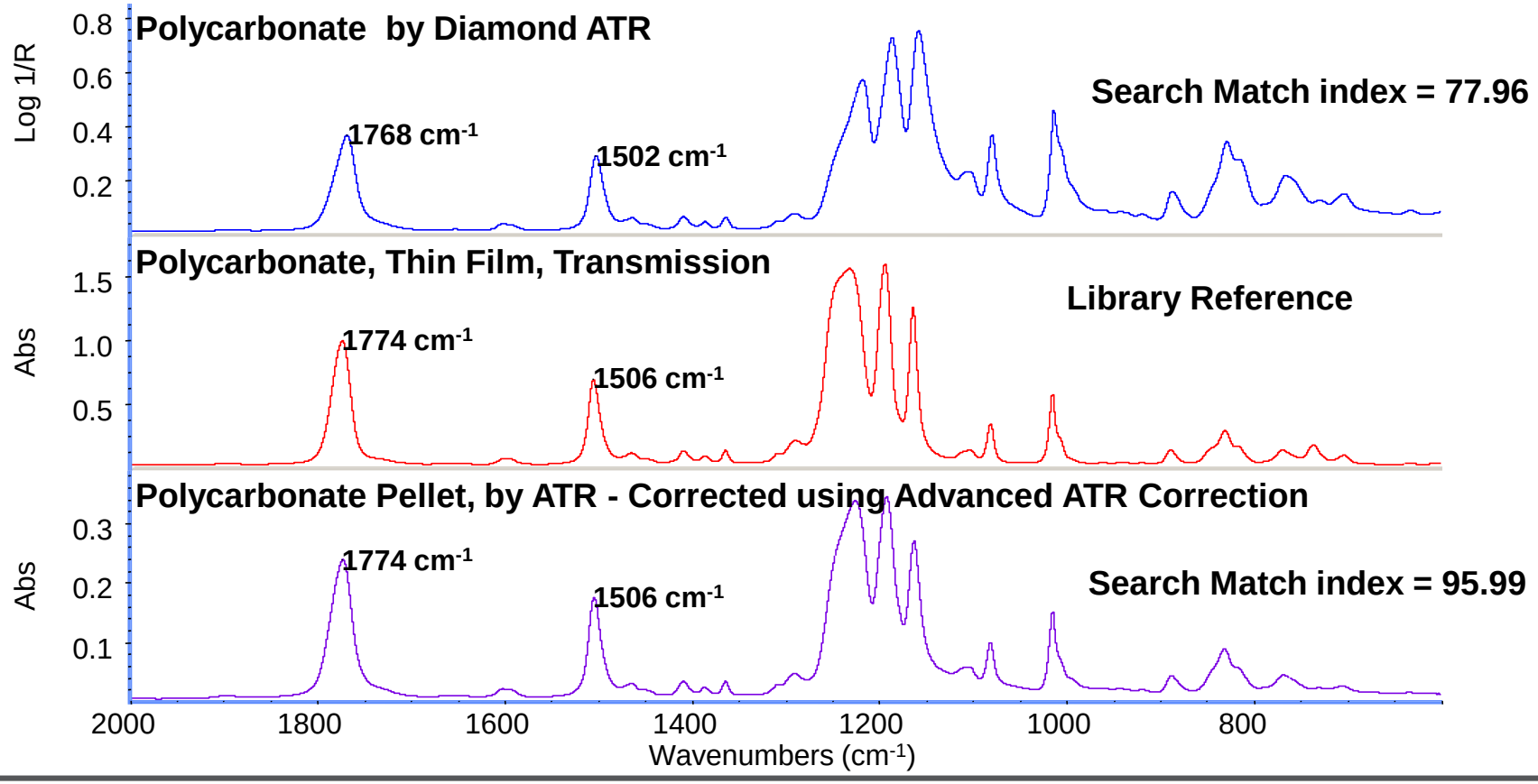
Converting ATR Spectra to Transmission-like Data for Better Library Match

The ATR peaks are altered by the complex interactions at the surface of the ATR crystal.

Advanced ATR Correction in OMNIC converts an ATR spectrum to a transmission-like spectrum using known math algorithm, improving the search results and agreement with databases of spectra.



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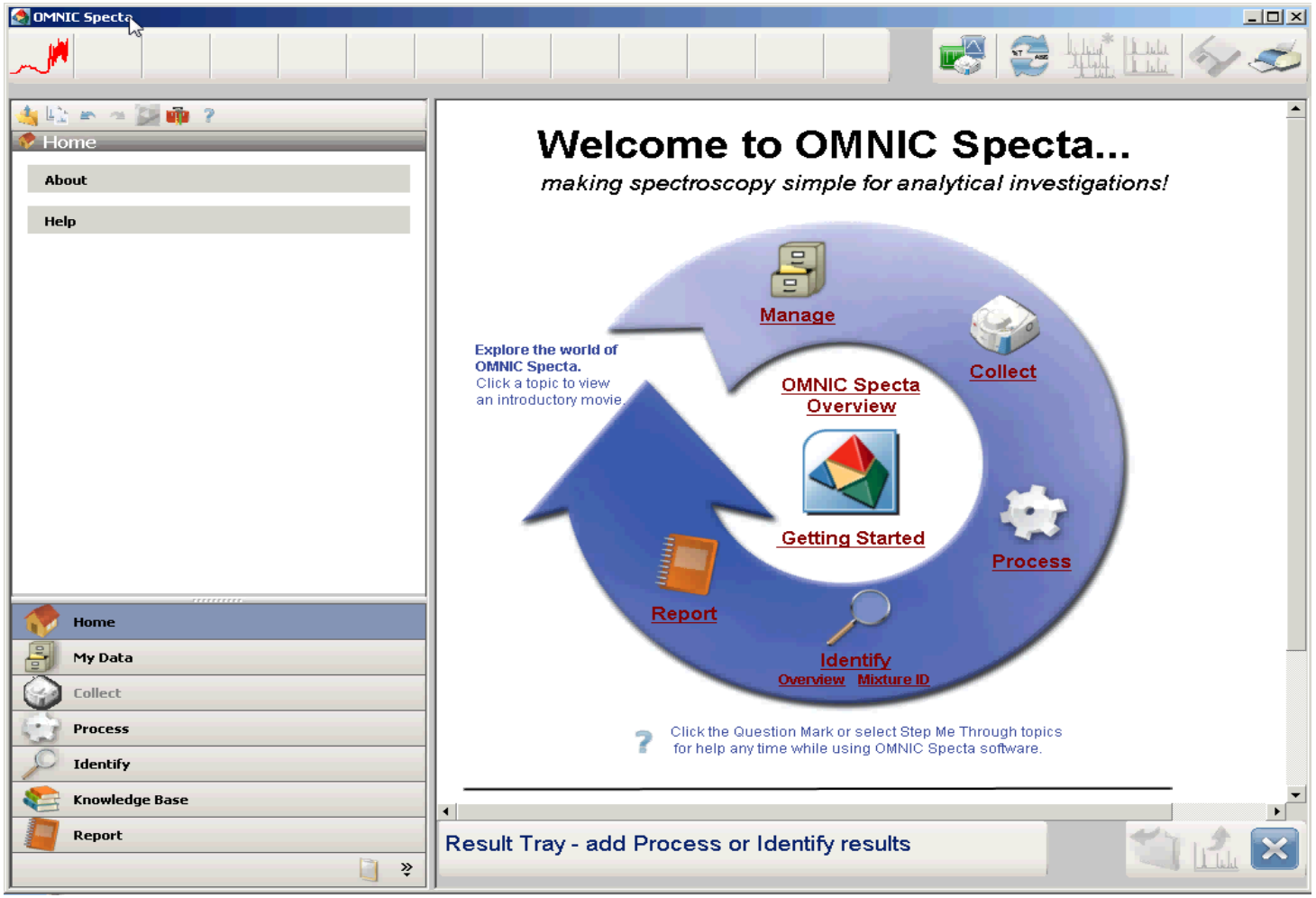
Material ID Library Search
Multi-Component ID Search

Multi-component Identification with OMNIC Specta

- Software for multi-component analysis of simple mixtures (identifies up to 4 compounds simultaneously in a mixture).



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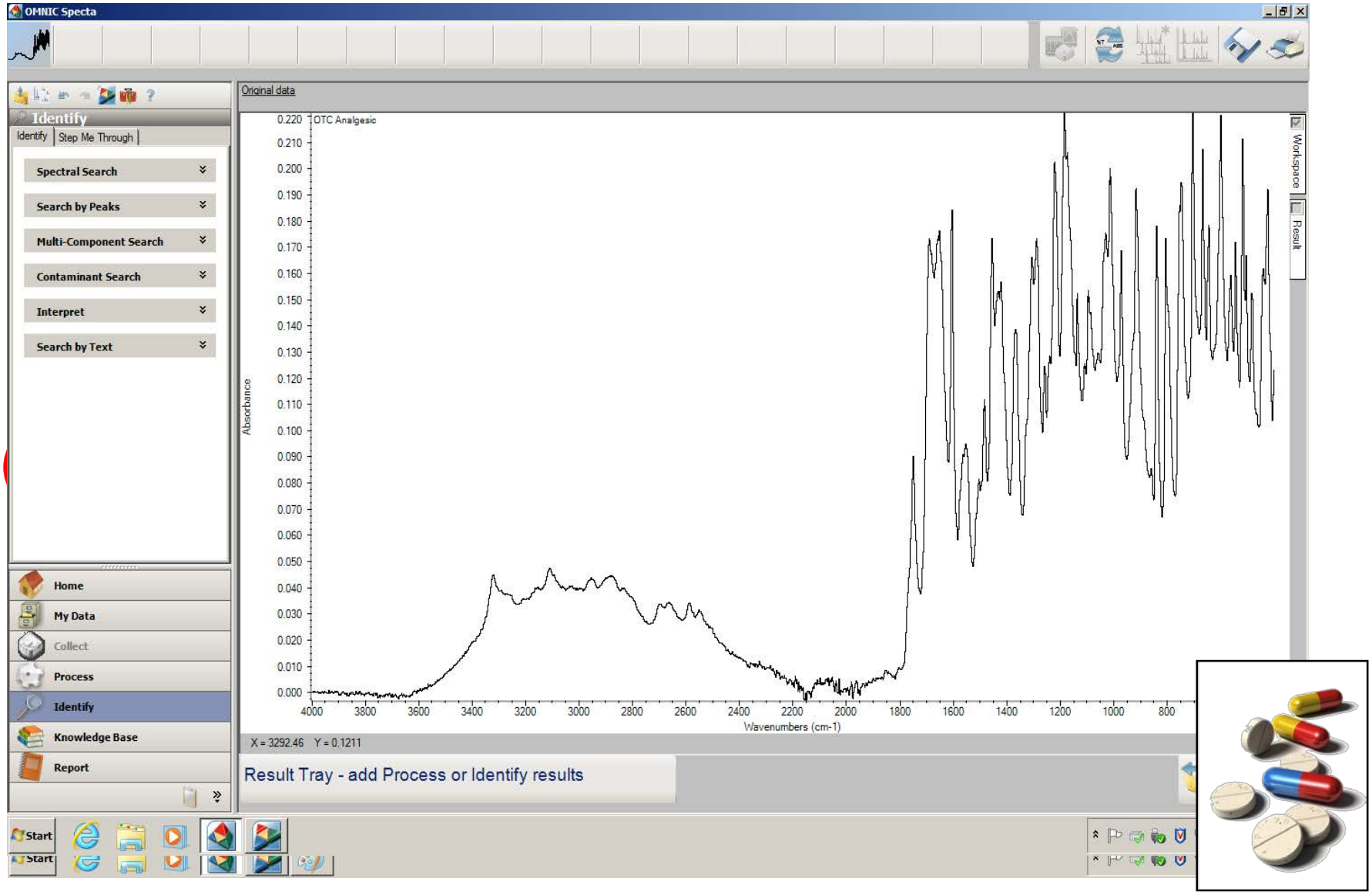
Multi-component Identification with OMNIC Specta



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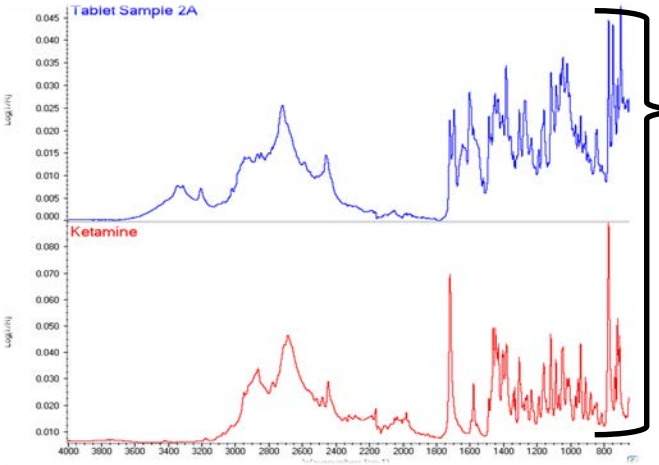
Drug Identification in the Forensics Laboratory



The spectrum of a suspicious substance was analyzed by OMNIC Specta into its components - it is not just ketamine – a four component mixture identified easily included methamphetamine and procain

	Match	Title	Cumulative	Composite%	Folder	Filename	Index
1	83.49	KETAMINE HCL	33.84	32.29	HR Comprehensive Forensic FT-IR Co...	c:\my docum...	1636
		d-Methamphetamine HCl by ATR	67.21	26.31	HR Comprehensive Forensic FT-IR Co...	c:\my docum...	1082
		PROCAINE HCl	79.83	19.06	HR Comprehensive Forensic FT-IR Co...	c:\my docum...	2907
		Vivarin Caffeine tablets	83.49	22.34	HR Comprehensive Forensic FT-IR Co...	c:\my docum...	3679

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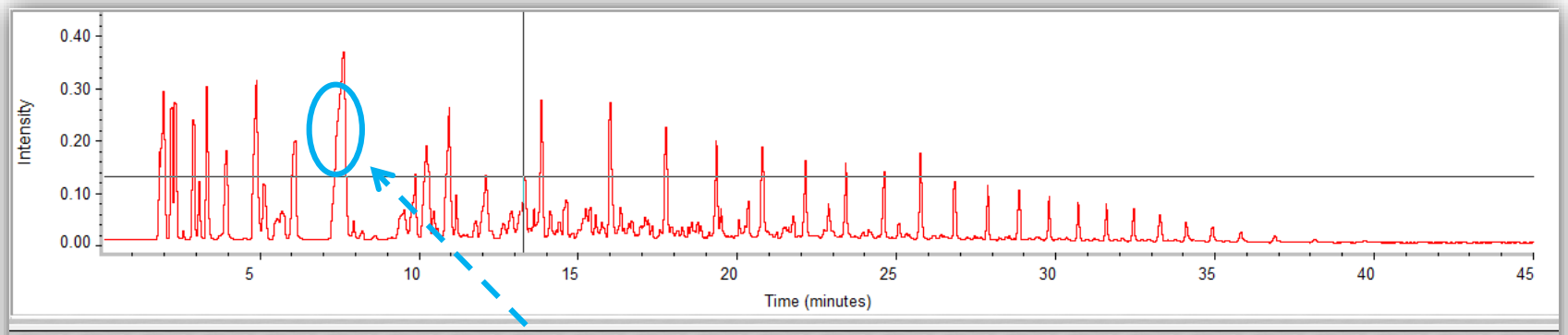
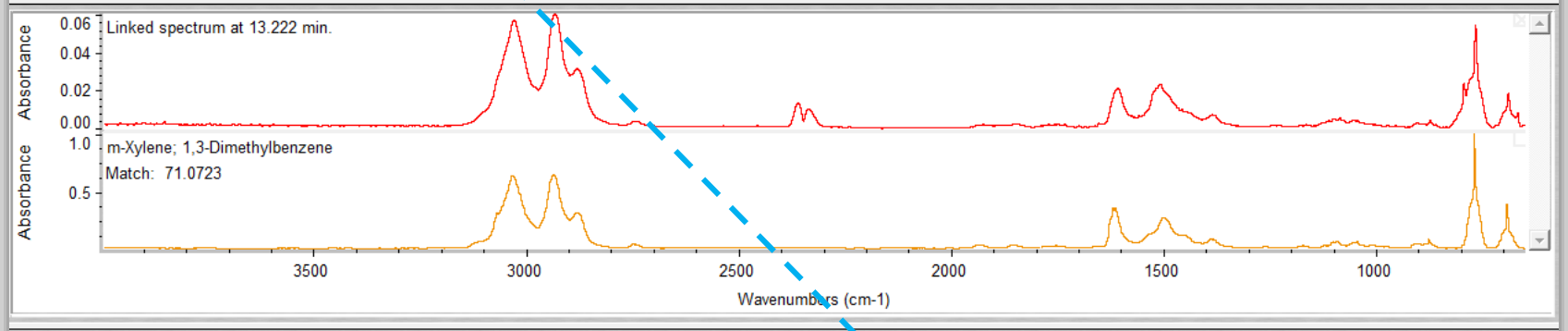
GC-IR Search

OMNIC Mercury Series GC-IR Identification





Retention Time	Match	Compound Name	Library Name	Index
8.1250	52.0531	Carbon dioxide	HR Nicolet Vapor Phase	3873
9.4314	78.1214	2-Methylheptane	HR Nicolet Vapor Phase	42
9.7819	87.1418	Toluene; Methylbenzene	HR Nicolet Vapor Phase	0
10.1324	89.0256	1,3-Dimethylcyclohexane, cis-	HR Nicolet Vapor Phase	
10.3873	60.1657	1,1-Dimethylcyclohexane	HR Nicolet Vapor Phase	
10.8652	93.2497	2-Aminooctane; 1-Methylheptylamine	HR Nicolet Vapor Phase	05
11.0883	74.3754	1,3-Dimethylcyclohexane, trans-	HR Nicolet Vapor Phase	235
11.6937	70.6362	Mineral spirits; Ligroin	HR Nicolet Vapor Phase	34
12.0123	94.0005	Propylcyclohexane	HR Nicolet Vapor Phase	220
12.5540	55.2237	Guaiene; 1,4-Dimethyl-7-isopropylidene-1,2,3,4,5,6,7,	HR Nicolet Vapor Phase	343
12.8089	80.9681	2-Methyloctane	HR Nicolet Vapor Phase	45
13.2231	71.0723	m-Xylene; 1,3-Dimethylbenzene	HR Nicolet Vapor Phase	4421
13.5417	77.5364	2,6-Dimethylcyclohexanemethanol	HR Nicolet Vapor Phase	1005
13.7648	92.1922	Nonane	HR Nicolet Vapor Phase	10
14.0197	76.1310	2-Aminooctane; 1-Methylheptylamine	HR Nicolet Vapor Phase	1705
14.3383	66.4692	Butylcyclopentane	HR Nicolet Vapor Phase	217

1. **Co-adds spectra**
2. **List peaks by retention time**
3. **Identifies separated substances**

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Conclusion FT-IR and Raman Spectral Databases

- Thermo Nicolet high quality commercial collections of FT-IR and Raman Spectral Libraries encompassing some 258,000 compounds are available

- IR Databases or Libraries created using accessories for ATR – Attenuated Total Reflection AND Transmission via Films, Mulls, Liquid cells and Pellets

- Sample spectra collection. Parameters are important to consider when analyzing your unknown or known standard for creation of your own library databases. Spectral Resolution, Number of scans and spectral data processing certainly affect the quality of a database search.

  Spectral range to collect your samples can lead to better confidence in a database result - 4000 to 400 Mid-IR, 12000 to 2800 Near-IR, 700 to 10 Far-IR and 4000 to 50 for Raman spectra

- OMNIC Software products to easily identify functional groups, unknowns and for multi-component identification.

Q & A