

Analyze IQ[®] Spectra Manager:

Store, Organize, and Link Your Spectral Data

Analyze IQ Spectra Manager allows you to store and organize valuable chemical spectra and associated information, and has a modern, easy-to-use interface.

Your spectra are valuable assets: **Spectra Manager** makes it easy for you to store and organize the spectra and related meta-data. You can build up an in-house library of spectra or use it with third-party libraries. It even gives you direct access to **linked data from the web**.

Spectra Manager is the ideal alternative to the high cost and effort of implementing a LIMS, or the all-too-common approach of keeping spectra in spreadsheets or folders, where associated information and context would be lost.

Acetonitrile:Methanol:Water(30:50:20) - Mixture Sample

Spectral Acquisition Details

The items in blue cannot be changed.
You can edit items in black and press 'Update Spectrum'.

Spectrum filename: MP28JULY2006-L12.SP
Date of collection: 28/07/2006
Time of collection: 12:28

Number of spectra collected: 1
Instrument model: RamanStn
Wavenumber range sampled:
Minimum: 250.0
Maximum: 3200.0
Number of data points: 1476

Collected by: Marissa Phelan
Spectral acquisition time (secs.): 21
Scans acquired per spectrum: 21
Axis labels: X: Raman Shift (cm-1)
Entered in database by: Lena Karlson
Entered date: 30/11/2006

Log Details

Analyze IQ Spectra Manager

File Libraries Help

Spectrum List

Raman data in Analyze IQ Full Raman Library

(Find by name)

ID	Type	Constituents
2263	Mixture	Acetonitrile; Methanol...
2265	Mixture	Acetonitrile; Methanol...
2266	Pure	Acetic acid, ammonia...
2269	Mixture	Acetonitrile; Methanol...
2271	Mixture	Acetonitrile; Methanol...
2272	Pure	3-Pyridinecarboxamide
2273	Mixture	Acetonitrile; Methanol...
2274	Mixture	Acetonitrile; Methanol...
2275	Mixture	Acetonitrile; Methanol...
2277	Pure	3-Pyridinecarboxylic a...
2278	Mixture	Acetonitrile; Methanol...
2279	Mixture	Acetonitrile; Methanol...
2280	Pure	1H-Indene-1,3(2H)-di...
2281	Mixture	Acetonitrile; Methanol...
2283	Pure	Benzenamine, 4-nitro...
2285	Pure	2-Butenedioic acid (2E)
2286	Mixture	Acetonitrile; Methanol...
2288	Mixture	Acetonitrile; Methanol...
2291	Mixture	Acetonitrile; Methanol...
2292	Mixture	Acetonitrile; Methanol...
2294	Pure	1,2,3-Propanetricarbo...
2301	Pure	D-Glucose
2302	Pure	1-Hexadecylamine...
2303	Pure	1,3-Propanediol, 2-am...
2304	Mixture	Acetonitrile; Methanol...
2307	Mixture	Acetonitrile; Methanol...
2308	Mixture	Acetonitrile; Methanol...
2309	Pure	2-Propenoic acid, 2-m...
2310	Mixture	Acetonitrile; Methanol...
2311	Pure	Guanidine, hydrochlor...

Acetonitrile:Methanol:Water(30:50:20)

Intensity

Raman Shift (cm-1)

Acetonitrile:Methanol:Water(30:50:20)

Details from Wikipedia

Select a constituent to see its details

IUPAC Name	Conc.	Common	CAS No.	Wikipedia
Acetonitrile	30%	Acetonitr...	000075-05-8	Acetonitrile
Methanol	50%	Methanol...	000067-56-1	Methanol
Water	20%	Water	007732-18-5	Properties, o...

Details for Acetonitrile

Acetonitrile

CC#N

Molecular formula: C₂H₃N
Molar mass: 41.05 g mol⁻¹
Appearance: Colorless liquid
Density: 786 mg mL⁻¹
Melting point: -46 to -44 °C; -51 to -47 °F; 227 to 229 K
Boiling point: 81.3 to 82.1 °C; 178.2 to 179.7 °F; 354.4 to 365.2 K
Solubility in water: Miscible
log P: -0.334
Vapor pressure: 9.71 kPa (at 20.0 °C)
K_H: 530 μmol Pa⁻¹ kg⁻¹
Acidity (pK_a): 25
Basicity (pK_b): -11
λ_{max}: 195 nm
Absorbance: ≤0.10

Spectra Manager integrates with **Analyze IQ Lab**, so that you can easily select appropriate spectra from which to build Analyze IQ models.

Spectra Manager also integrates with **Analyze IQ SmartSearch**, so that you can identify best matches for unknown spectra, quickly and reliably.

Download a free evaluation of Spectra Manager
at www.AnalyzeIQ.com



Analyze IQ Spectra Manager is part of the Analyze IQ product suite, which is the world's most advanced chemometrics and spectroscopy analysis software.

Spectra Manager is the spectral library and data management package that allows you to store and organize spectra and their related meta-data, easily and efficiently.

Its features include:

- ◆ Browse spectra and switch between spectrum details, constituent details, plots of spectra, and data from the web
- ◆ Store CAS registry numbers and QA details
- ◆ For each sample, record important details such as the manufacturer, catalog number, lot number, date opened, and purity
- ◆ Full-text search and listing of spectra by IUPAC and common names.
- ◆ For mixtures, all the relevant data can be included, so that you can track mixtures that use the same materials by lot numbers.

With **Spectra Manager** you can insert spectra into libraries and remove them, and select any entry to view its spectrum and edit associated data, such as lot number, manufacturer, appearance, IUPAC name, common name, and so on.

Details for Methanol

Constituent details can be changed, except for the Manufacturer

CAS # 000067-56-1

IUPAC Name Methanol

Common Names List: Bieleski's solution, Carbinol, Methanol cluster, Methyl alcohol, Methyl hydroxide

Buttons: Insert, Update, Delete

Manufacturer: BDH

Catalog Number: 29192BL

Lot Number: K31794469

Date Opened: 24/07/2006

Purity: 99.5%

Location: Phys Chem

Spectra Manager links seamlessly with **Analyze IQ Lab**, allowing users to select data from their database for the development of Analyze IQ models. Functionality is provided to **auto-select** the training set, by scanning the databases for all samples that include the target material and other relevant samples, such as those that contain materials that occur in mixtures with the target material.

It also links seamlessly with **Analyze IQ SmartSearch**, with which you can search quickly and accurately through your library of spectra, to identify the best matches for a query spectrum.

A **unique feature** of **Analyze IQ Spectra Manager** and **SmartSearch** is that they can display **linked data from Wikipedia** associated with your data.

Details for Acetic acid

Acetic acid

Chemical structures: CC(=O)O, CC(=O)O

Properties

Molecular formula	C ₂ H ₄ O ₂
Molar mass	60.05 g mol ⁻¹
Appearance	Colourless liquid
Odor	vinegar-like
Density	1.049 g cm ⁻³
Melting point	16 to 17 °C; 61 to 62 °F; 289 to 290 K
Boiling point	118 to 119 °C; 244 to 246 °F; 391 to 392 K
Solubility in water	Miscible
log P	-0.322
Acidity (pK _a)	4.76
Basicity (pK _b)	9.198
Refractive index (n _D)	1.371
Viscosity	1.22 mPa s
Dipole moment	1.74 D

Thermochemistry

Works with Multiple Libraries:

- ◆ Analyze IQ Raman Spectra Library
- ◆ Third-party commercial libraries
- ◆ Build up your own libraries in-house
- ◆ Keep libraries on one machine or share them in your department
- ◆ We can assist you in importing your spectra or legacy data.

Library Selection

Name	Type	Supplier	Valid From	Valid Until
ANIQ_RAMAN_FULL	Raman	Analyze IQ	2001-Jan-01	Perpetual
MM_TEST_NMR	NMR	User	2013-Jan-01	Perpetual
MM_TEST_RAMAN2	Raman	User	2013-Jan-01	Perpetual

Library: Analyze IQ Full Raman Library.

Description: Dataset of 1868 Raman spectra of common organic materials (pure materials and mixtures), including the exact composition of each material and all associated data.

Buttons: Select, Activation, License Info, OK, Cancel

Popular file formats are supported:

- ◆ SPC: Thermo-Fisher's GRAMS SPC format
- ◆ SpectroML: NIST's XML-based format
- ◆ AIQ: format used in the Analyze IQ software suite
- ◆ JCAMP-DX: IUPAC's popular JCAMP-DX file format
- ◆ XY Text Files and CSV Files

