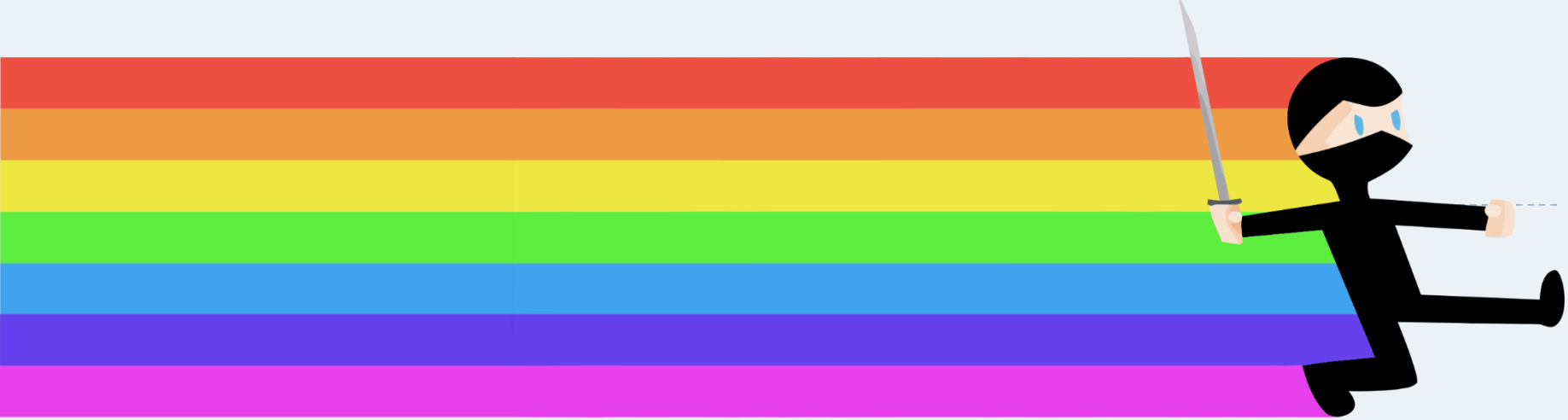


http://spectroscopy.ninja

Spectroscopy Ninja

Optical Spectroscopy Software Development

Proudly presenting:

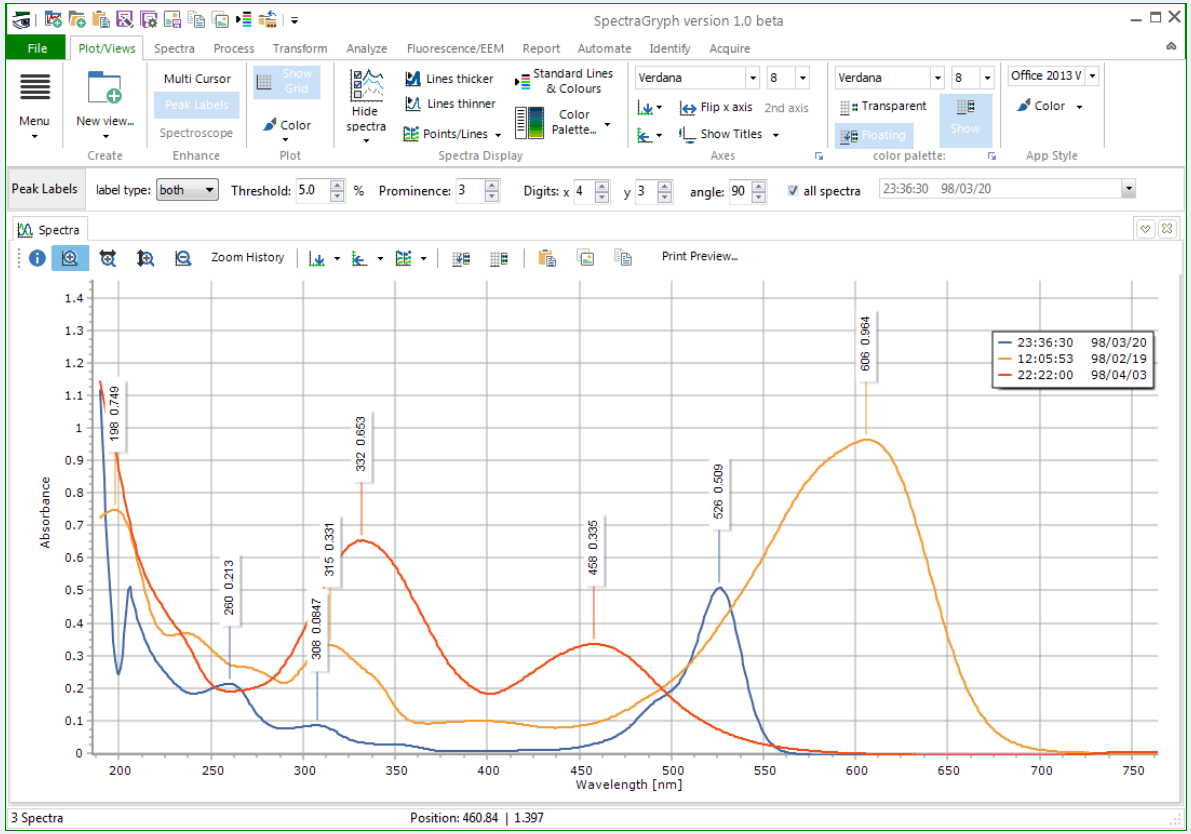
About 10 pages	Features 22 pages	Testimonials 2 pages
	Links (1 page)	Applications (3 pages, growing)

SpectraGryph

... ONE APP TO TREAT THEM ALL ...

What it is:

- Universal software for optical spectra processing
- Easy to use
- Rock solid
- Lean
- Free for private & academic use (in standard version)



What it improves:

- Frees the data from the instrument computer
- Brings all kind of spectra together
- To visualize/ analyze multiple spectra at once
- One processing solution for all file formats

What it does:

- Open UV-VIS, NIR, FTIR, Raman, fluorescence, LIBS, XRF
- 70 file formats recognized
- View, analyze, process & convert many spectra *in parallel*
- Automated batch processing with predefined sequence
- Spectral database search & matching
- Live spectra acquisition & spectrometer control

Who does it:

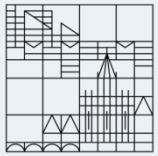
- Dr. Friedrich Menges
- studied chemistry 1993-1999
- 2000 – 2005: PhD in physical chemistry
- 2005-2010 device developer for minia-
- turized/ microfluidic bioanalytical systems
- 2010-2016: R&D system engineer (Tecan/Salzburg), developing multi-mode microplate readers
- Since June 01, 2016: full-time with Spectroscopy Ninja

- 2000 – now: spectroscopy software development

Where it comes from:

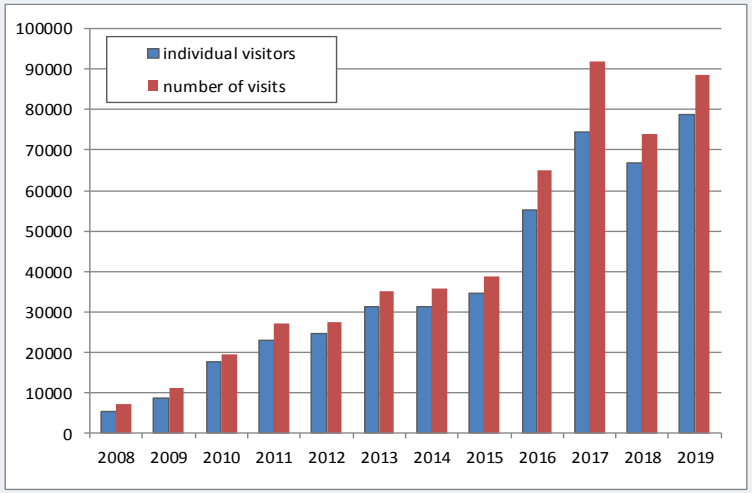
- 2000 – 2005: PhD at Universität Konstanz
- initially: **Spekwin32** as tool for internal use
- late 2002: first web site
- 03/2004 : english version
- 2010: dual use conditions, trade license
- 08/2014: creation of Spectroscopy Ninja
- June 01, 2016: full-time with Spectroscopy Ninja (as a single person)

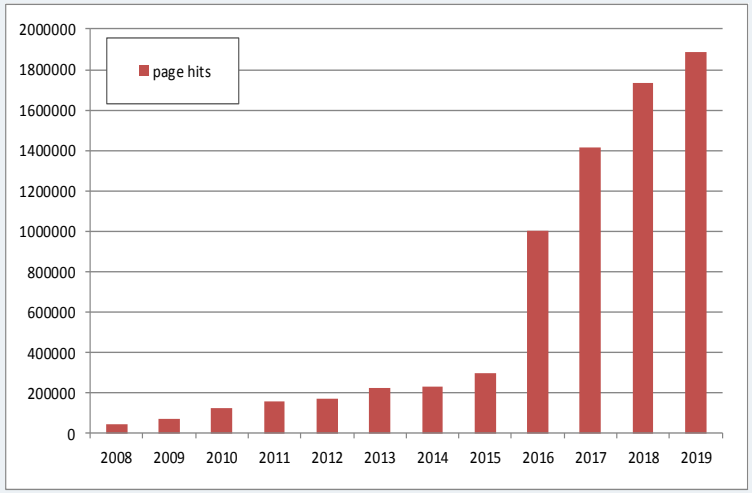
Universität Konstanz

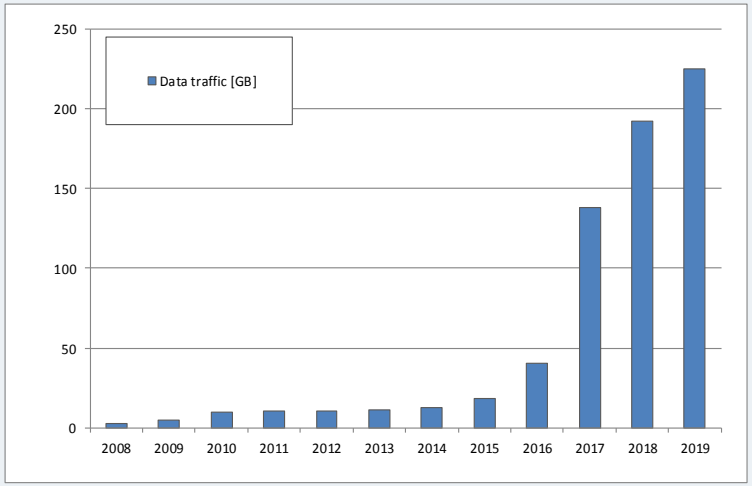


- Nov 11, 2016: release of **Spectragryph** as modernized, enhanced successor software for the outdated Spekwin32

Where it is g(r)o(w)ing to:







as of 12/2019:

- 42,000 downloads since first release
- 25 software updates released
- 3 major areas added (identification, automation, acquisition)
- 30 new file formats recognized

What to pay for it:

Spectragryph variant	Non-commercial use	Academic distribution	Commercial use
Spectragryph *standard version*	**Free**	**€ 500**	**€ 290**
Spectragryph-on *modular spectrometer control*	**€ 125**	**€ 2900**	**€ 590**
Spectragryph-id *unlimited spectral database search*	**€ 200**	**€ 4400**	**€ 790**
Spectragryph-id-on *database search & spectrometer control*	**€ 290**	**€ 6500**	**€ 990**

Licenses are valid forever with no recurring costs, include all future updates!

Who paid for it:

Which industries:

- Optics, Lasers, Spectroscopy
- Analytical Instrumentation
- Chemicals, Materials
- Pharmaceuticals
  Life Sciences, Medical Devices
- Oil & Lubricants
- Mining, Exploration, Geology
- Gemmology, Gem Appraisal
- Arts & Conservation

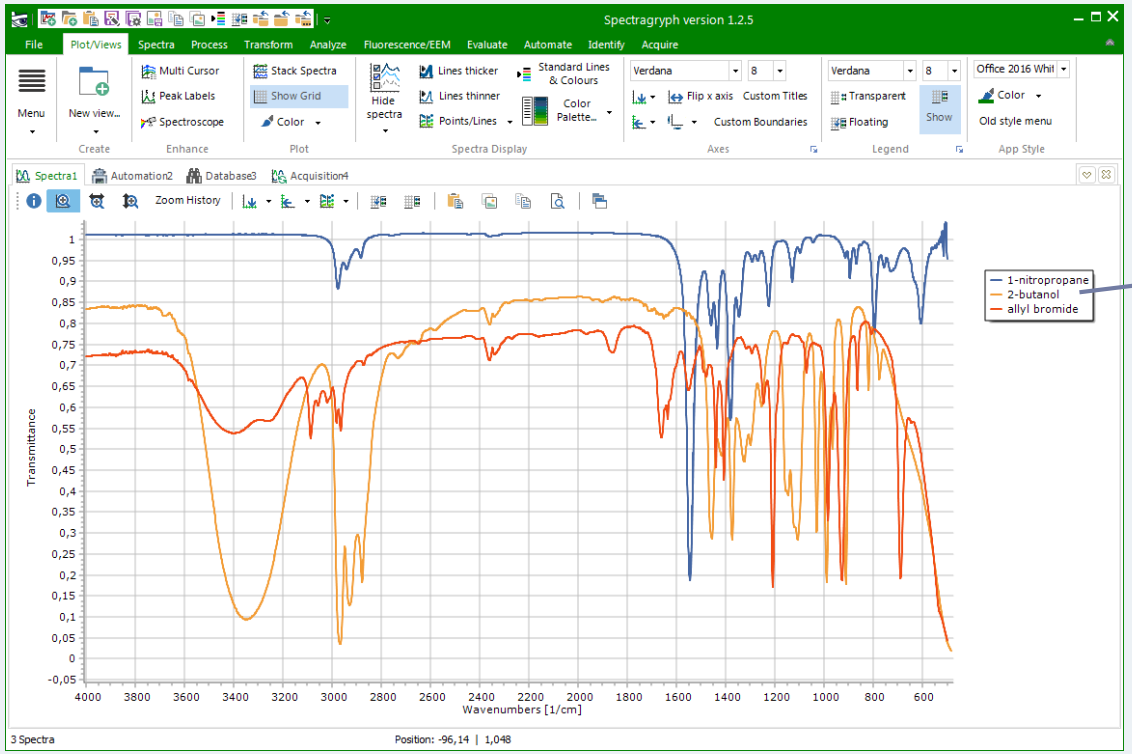
- & Academia, of course!
  (>200 Spectragryph citations, 450 alltogether)

Features: overview

User interface	Main window	Plot view	Spectra display
Data in/out	File formats	Process: baseline	Process: smoothing
Process: scaling	Process: removal	Process: chemometrics	Transform
Transform: new types	Analyze: peaks, integrals	Analyze: calculations	Analyze: extract data
Fluorescence/EEM	Automate	Identify: database creation	Identify: search results
Acquire			

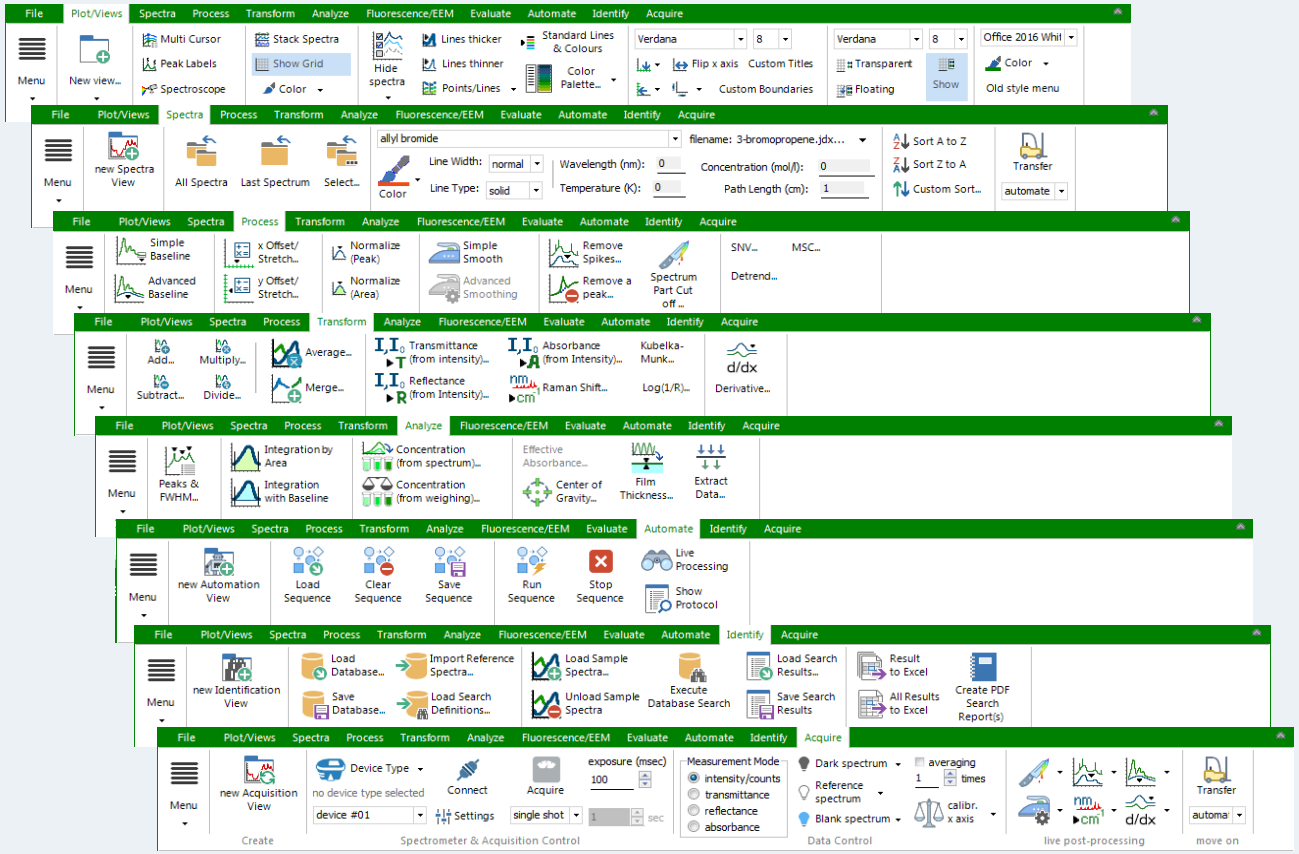
Features: user interface

- one main window: the plot
- arranged in browser-like tabs
- special tab types: EEM, identification, automation, acquisition

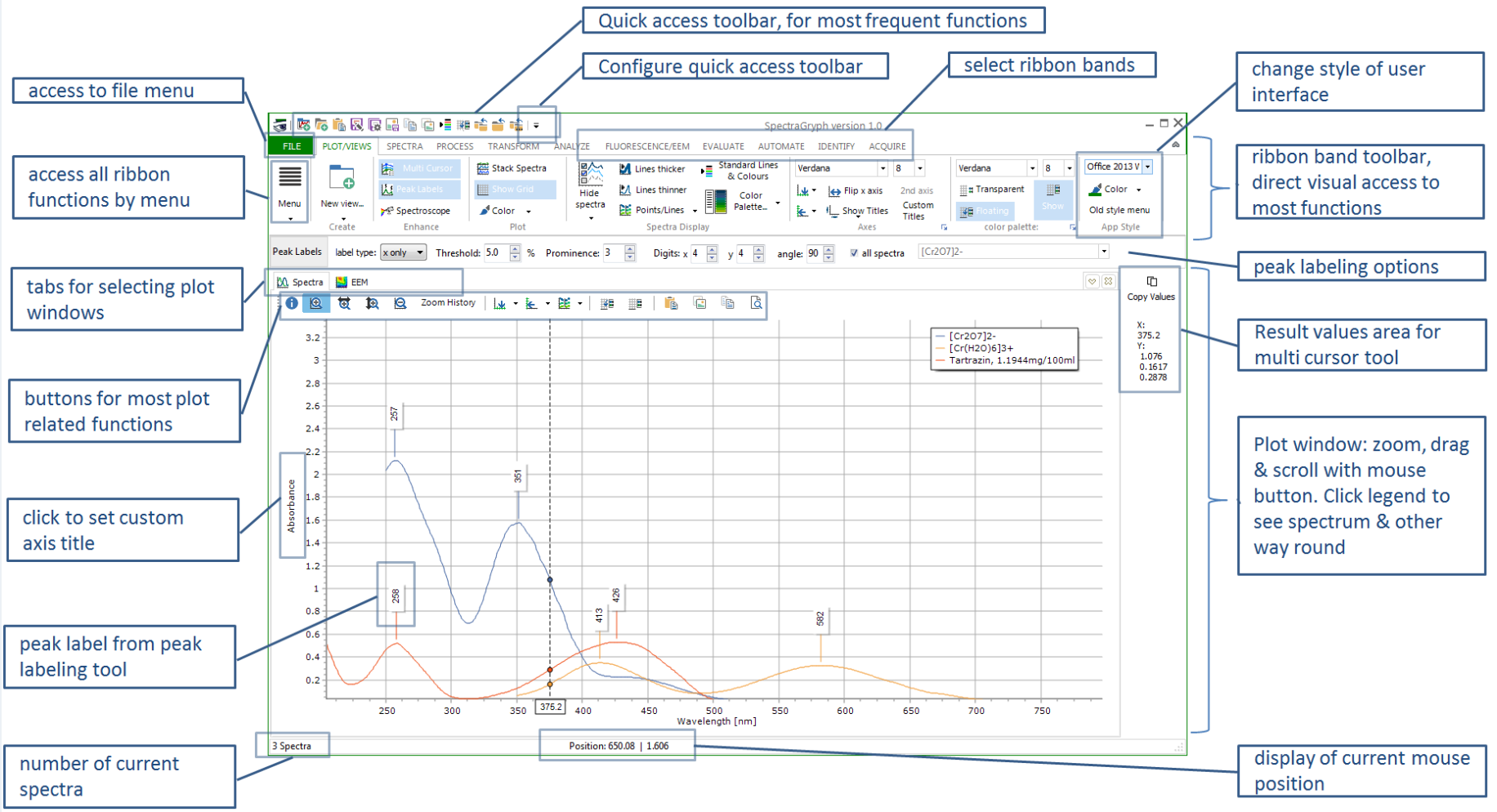


Features: ribbons

- All functions organized in ribbons (like Word, Excel, …)
- special ribbons for special function areas

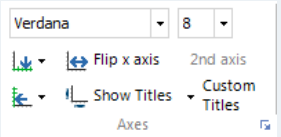


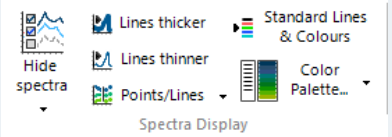
Features: all main window functions

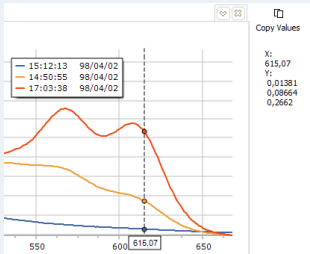


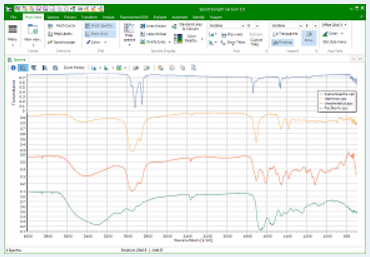
Features: controlling plot view

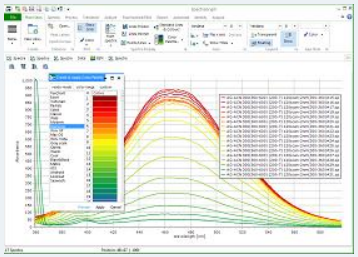
- On-the-fly x, y axis transformation
- Show/hide spectra, legend, grid, peak labels
- Select colour schemes, line thickness, text properties
- Set custom axis labels, locked axis ranges
- Zoom, unzoom, pan, scroll plot with mouse
- Stack spectra
- Special functions:
  - multi-cursor
  - spectroscope view

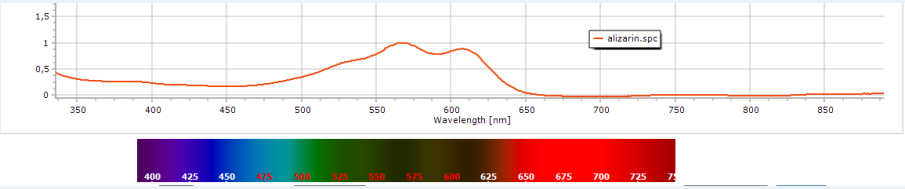


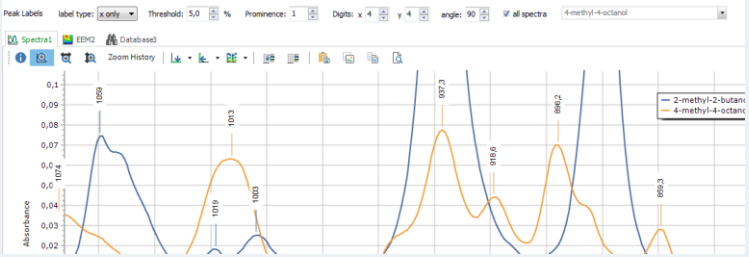






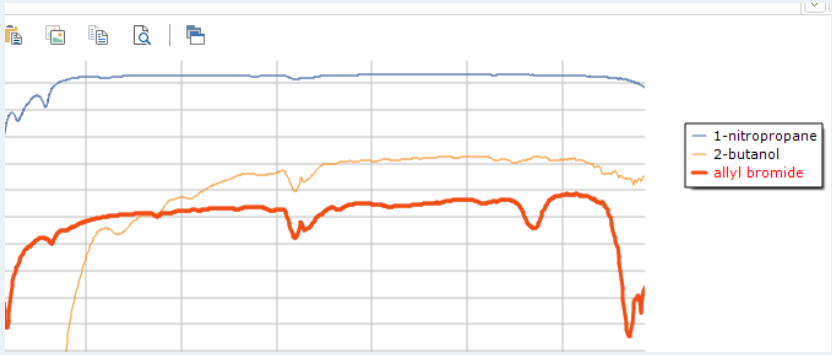






Features: controlling spectra display

- Set individual line properties, color
- Set spectrum properties, legend text (F6 short key)
- Sort A→Z or vice versa
- Select indiv. spectra from ribbon
- Click legende text to highlight spectrum (& vice versa)
- Shift&scale individual spectra
- Undo
- Delete all, last or a selection
- CTRL+Click on spectrum for direct delete



Features: data input/output

- Open all recognized file formats with File→Open
- Drag&drop files into plot window from explorer
- Copy&paste data columns from Excel or text editor
  ➔ will be recognized as spectrum plot

- Save spectra as 8 data formats (spc, dx, nir, csv, dat, sgd, spv, rruff)
- Batch export all spectra into 5 file formats
- Copy data tables to clipboard
- Save plot as 7 picture formats (bmp, emf, eps, pdf, png, svg, wmf)
- Copy plot picture to clipboard (as vector graphics)

Features: file formats

- Reading original binary files & exported spectral data from these manufacturers:

AIT/ Analect

Agilent

Princeton Instruments

StellarNet Inc

ANDOR TECHNOLOGY

ascanis

COLVISTEC Inline Process Monitoring

EnSpectr Enhanced Spectrometry

analytikjena

SHIMADZU

ASD Inc.

BRUKER

GE

JASCO

RENISHAW

AVANTES enlightening spectroscopy

biochrom

NT-MDT Spectrum Instruments

PerkinElmer

Roper Technologies

B&W TEK INC.

HITACHI

Ocean Optics

ThermoFisher SCIENTIFIC

BECKMAN COULTER

HORIBA Scientific

VARIAN

MILTON ROY

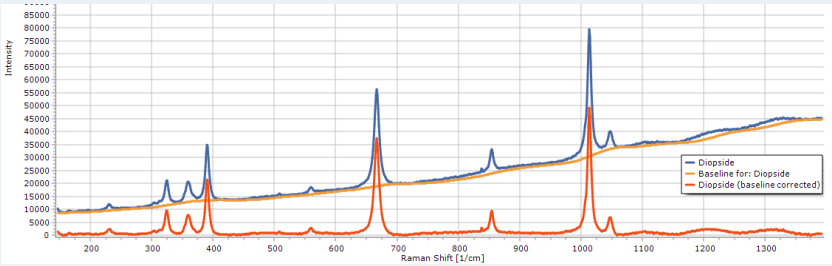
VWR

WTW

Features: Process (baselines)

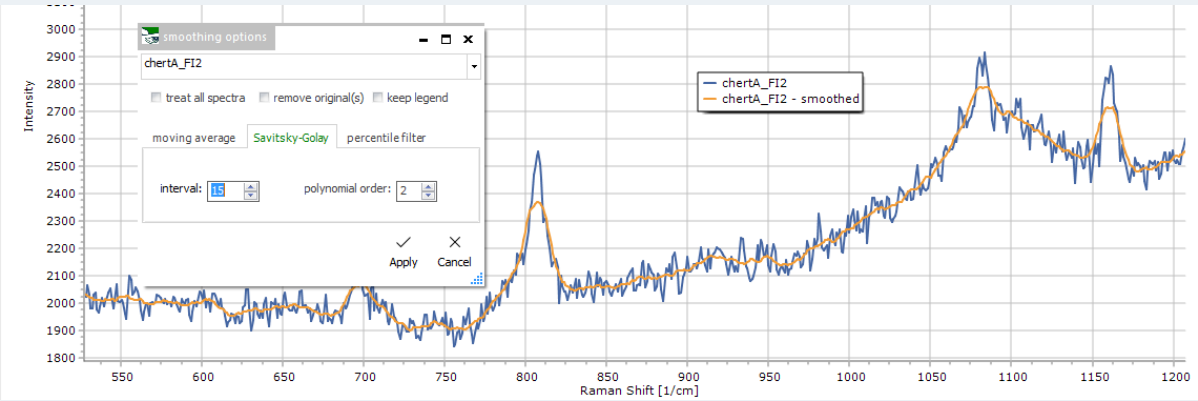
- *Simple baseline*: bring straight horizontal baseline down to zero (mainly UV-VIS, also Raman, LIBS)

- *Advanced baseline*: interactive baseline definition
  - *linear*: a linear baseline with variable slope & offset
  - *adaptive*: snuggling a curved baseline to spectrum bottom, best for Raman (fluorescence removal), FTIR, LIBS
  - *scattering*: mimicking a turbid solution's exponential baseline increase towards short wavelengths (UV-VIS only)



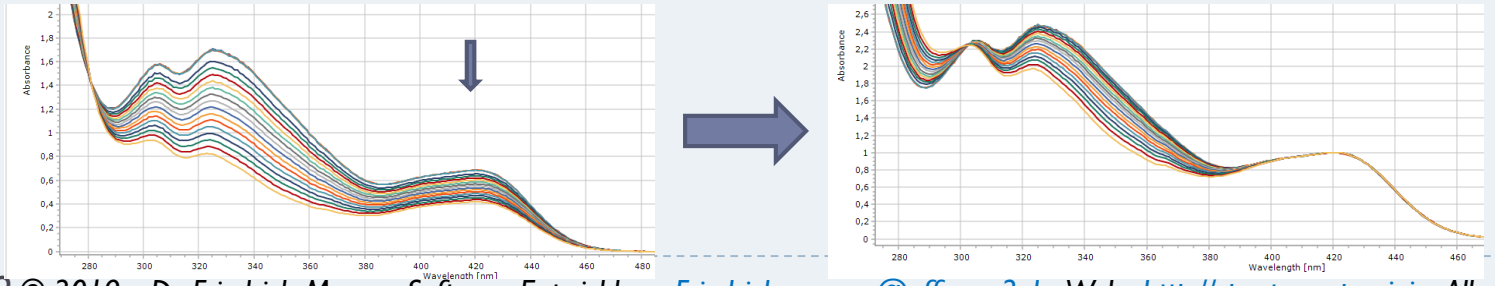
Features: Process (smoothing)

- *Simple smoothing*: with a Savitsky-Golay filter of medium strength, no settings
- *Advanced smoothing*: 4 algorithms with settings
  - *Moving average*: interval size, averaging function (rect. / triang.)
  - *Savitsky-Golay*: interval size, polynomial order (2nd – 5th)
  - *Percentile filter*: interval size, percentile (0 – 100%)
  - *Baseline selective*: vertical gradient, % of spectrum

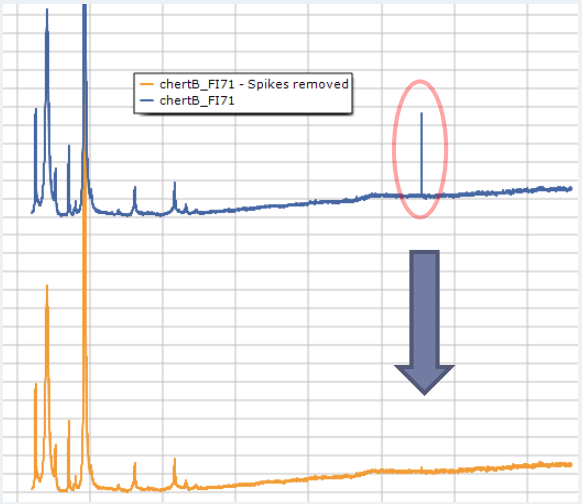


Features: Process (axes based)

- *x Offset / Stretch*: apply addition, subtraction, multiplication, division upon x axis values
- *y Offset / Stretch*: same upon y axis values
- *Normalize (Peak):*
  scale spectra, so that highest visible peak = 1
- *Normalize (area):*
  scale spectra, so that area under peak is the same
- *Normalize (value):*
  scale spectra to certain y value at certain x position



Features: Process (removals)



- *Remove Spikes*: removal of cosmic spikes, maximal width can be set. Useful for Raman, fluorescence (with long exp. times on Si-based detectors)

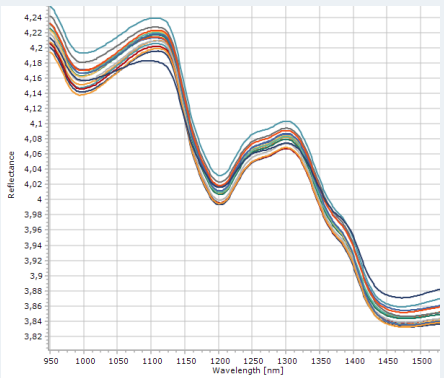
- *Remove a peak*:
  interpolate at a given position

- *Spectrum part cut off*:
  remove spectrum parts from both sides (start + end)

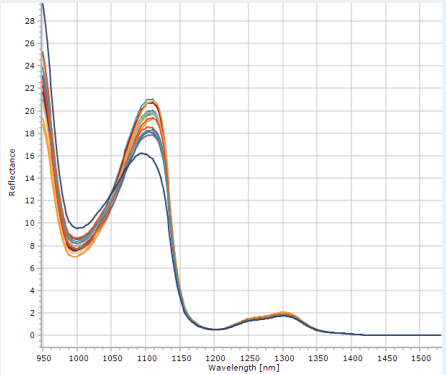
Features: Process (chemometr.)

Variability removal is often required in preprocessing of NIR spectrum series for chemometric applications

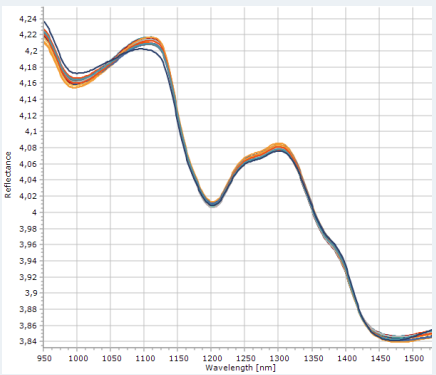
- *SNV*: standard normal variates
- *MSC*: multiplicative scatter correction
- *Detrending*: baseline detrending by subtracting polynom. fit



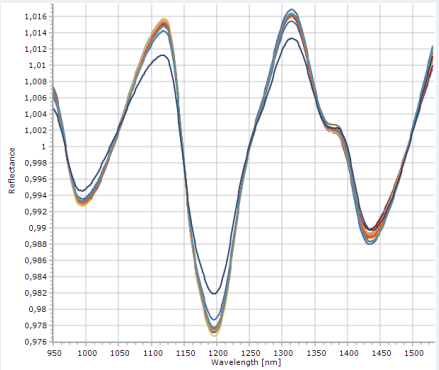
original



SNV



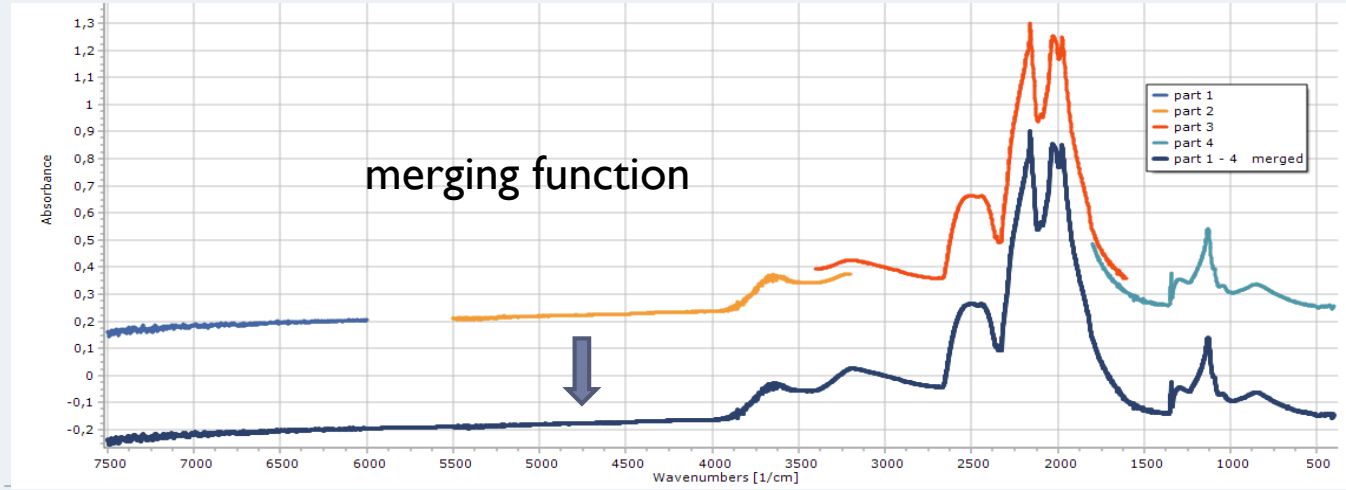
MSC



Detrending

Features: Transform

- Apply *addition, subtraction, multiplication, division* on spectra
- Interactive *scaled subtraction*
- *Average* a selection of spectra (selection rule set available)
- *Merge* a selection of spectra (selection rule set available)
- *Interpolate, resample* to new start/end value, step width
- Calculate 1st - 4th *derivative*, optional internal smoothing



Features: Transform (new types)

To create new spectrum types from given raw data:

Y AXIS:

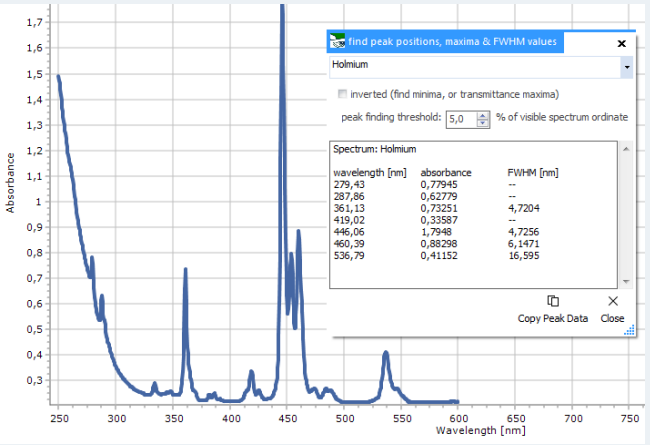
- *Transmittance* $\mathbf{T = I / I_0}$; *Reflectance* $\mathbf{R = I / I_0}$ (**I**: intensity)
- *Absorbance* $\mathbf{A = -1 * \log_{10}(T)}$
- *Kubelka-Munk* $\mathbf{K/S = (1 - R)^2/(2 * R)}$
- *Log(1/R)*: just this, for reflectance spectra

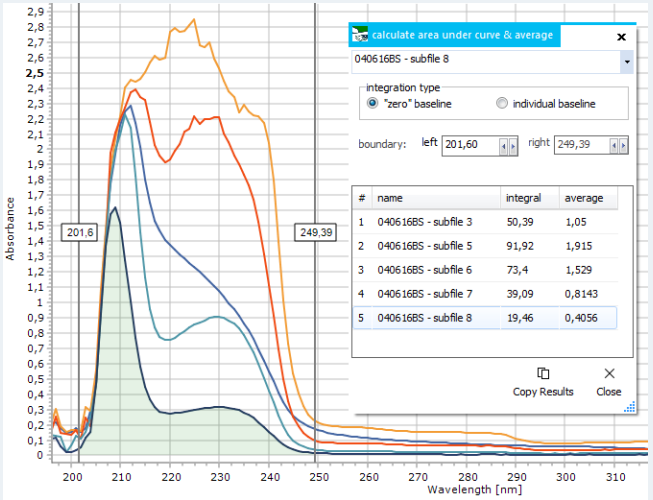
X AXIS:

- *Raman shift* $\mathbf{R = 10^7 * (1/\lambda_{laser} - 1/\lambda)}$, while R in cm^{-1}
- Apply *calibration*, for Pixels ➔ Wavelength, Wavenumbers

Features: Analyze (peaks, integrals)

- *Peaks & FWHM:*
  create a listing of peak positions & FWHM values & atomic emission line assignments (LIBS, XRF, Gamma)
- *Integration by Area*: create list of areas under peak for a defined x range (straigth baseline at zero)
- *Integration with baseline*: create a list of areas under peak for a defined x range (sloped, individual baseline)
- *Center of gravity*: weighted



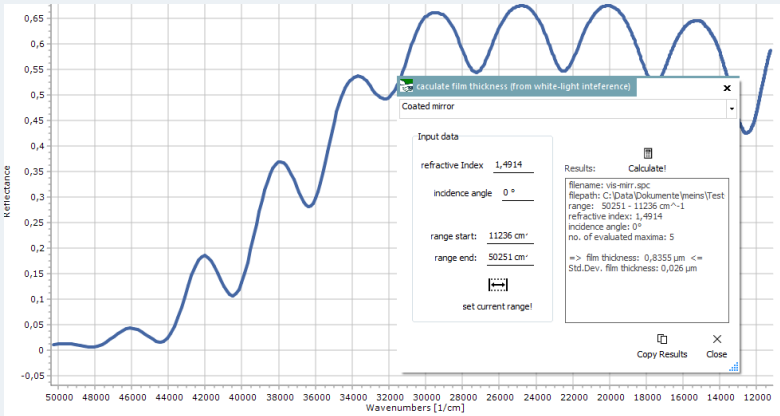


Features: Analyze (calculations)

- *Concentration: (from spectrum):* for UV-VIS spectra, use Lambert-Beer to calc. concentration values
  $\mathbf{E = \varepsilon * c * d \Leftrightarrow c = E / (\varepsilon * d)}$
- *Concentration: (from weighing):* calc. concentration values from sample weight, molecular mass and solvent volume

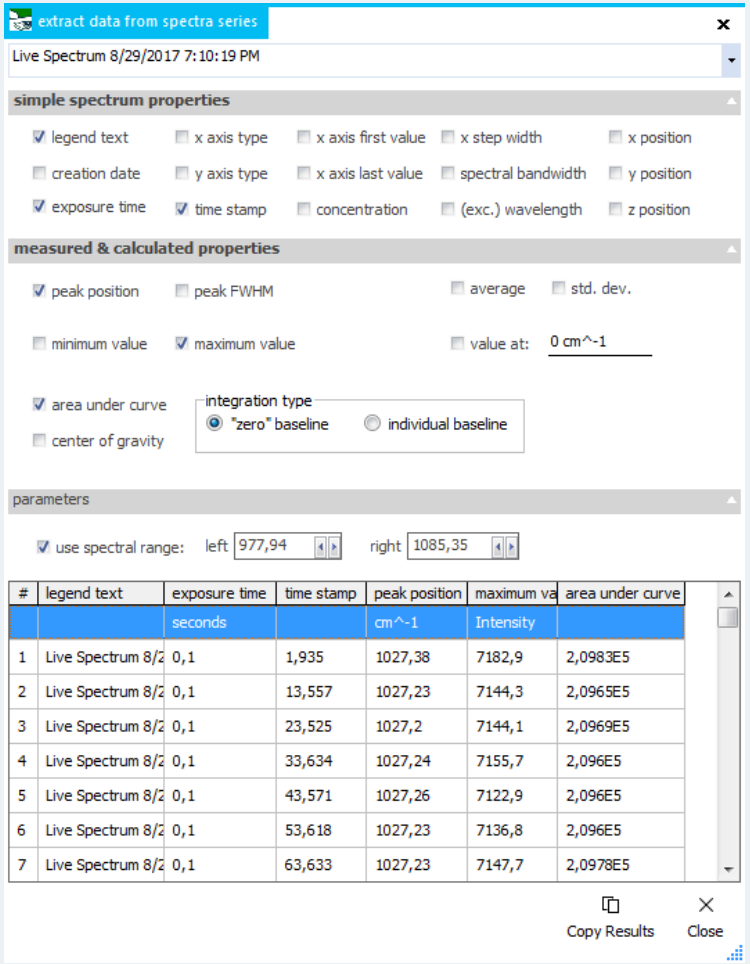
- *Film thickness*: calculated from fringes of white light interference spectrum. Input values: refractive index, incident angle, x axis range.

$$d = \frac{\Delta m}{2\sqrt{n^2 - \sin^2\theta}} \times \frac{1}{\left(\frac{1}{\lambda_2} - \frac{1}{\lambda_1}\right)}$$



Features: Analyze (extract data)

- Extract spectrum properties and calculated values for a series of spectra.
- Interactively define x axis range.
- Select from 24 parameters.
- Copy results list to clipboard

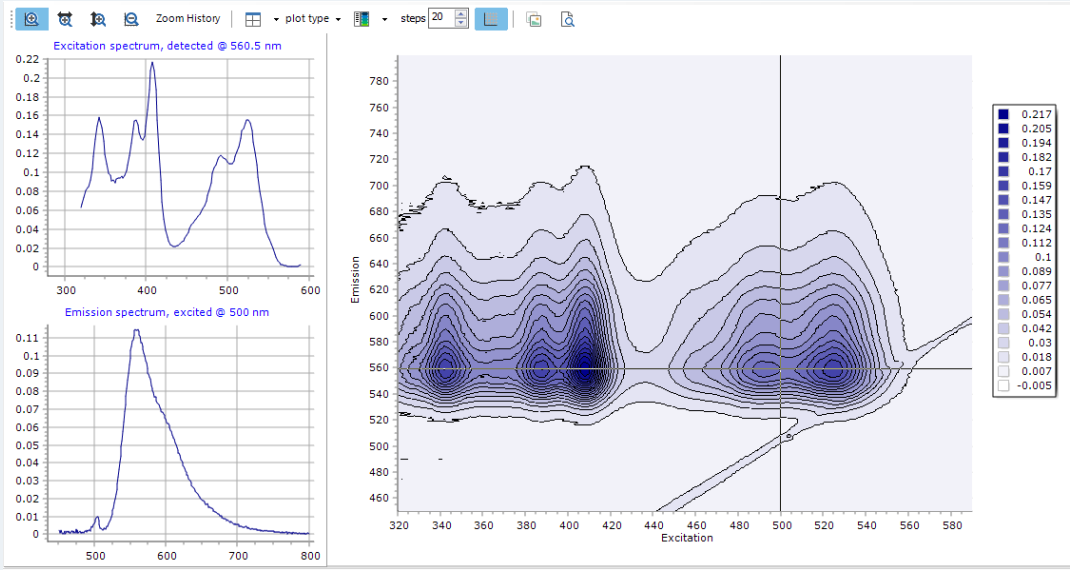


#	legend text	exposure time	time stamp	peak position	maximum va	area under curve
		seconds		cm^-1	Intensity	
1	Live Spectrum 8/2	0,1	1,935	1027,38	7182,9	2,0983E5
2	Live Spectrum 8/2	0,1	13,557	1027,23	7144,3	2,0965E5
3	Live Spectrum 8/2	0,1	23,525	1027,2	7144,1	2,0969E5
4	Live Spectrum 8/2	0,1	33,634	1027,24	7155,7	2,096E5
5	Live Spectrum 8/2	0,1	43,571	1027,26	7122,9	2,096E5
6	Live Spectrum 8/2	0,1	53,618	1027,23	7136,8	2,096E5
7	Live Spectrum 8/2	0,1	63,633	1027,23	7147,7	2,0978E5

	A	B	C	D	E	F	G
1	used spectral range:	977,94	to	1085,35			
2	#	legend text	exposure time	time stamp	peak position	maximum value	area under curve
3			seconds		cm^-1	Intensity	
4	1	Live Spectrum 8/29/2017 7:10:19 PM	0,1	1,935	1027,38	7182,9	1,32E+05
5	2	Live Spectrum 8/29/2017 7:10:31 PM	0,1	13,557	1027,23	7144,3	1,33E+05
6	3	Live Spectrum 8/29/2017 7:10:41 PM	0,1	23,525	1027,2	7144,1	1,33E+05
7	4	Live Spectrum 8/29/2017 7:10:51 PM	0,1	33,634	1027,24	7155,7	1,32E+05
8	5	Live Spectrum 8/29/2017 7:11:01 PM	0,1	43,571	1027,26	7122,9	1,32E+05
9	6	Live Spectrum 8/29/2017 7:11:11 PM	0,1	53,618	1027,23	7136,8	1,32E+05
10	7	Live Spectrum 8/29/2017 7:11:21 PM	0,1	63,633	1027,23	7147,7	1,33E+05
11	8	Live Spectrum 8/29/2017 7:11:31 PM	0,1	73,648	1027,21	7155,9	1,33E+05
12	9	Live Spectrum 8/29/2017 7:11:41 PM	0,1	83,648	1027,21	7149,6	1,33E+05

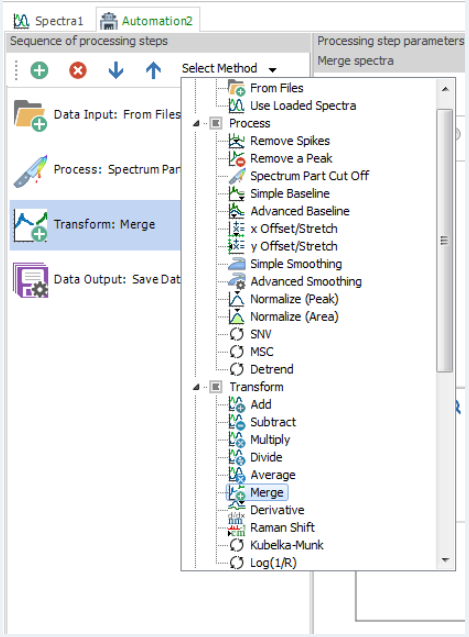
Features: Fluorescence/EEM

- Correct emission sensitivity & excitation intensity
- Assign excitation wavelengths
- Remove 1st & 2nd order Rayleigh and Raman scatter
- Subtract Blank datasets from EEM matrix
- Calculate excitation spectra
- Show:
  2D & 3D EEM plots
  with Ex & Em
  cross-sections

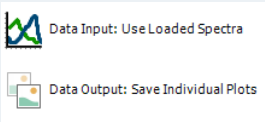


Features: Automate

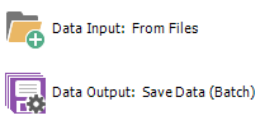
- Define sequences of processing steps
- Select from **45** possible steps
- Save sequence for further use
- Execute sequence on loaded spectra
- Execute sequence w/o showing spectra
- Turn live processing on/off
- Interrupt sequence execution
- With processing protocol



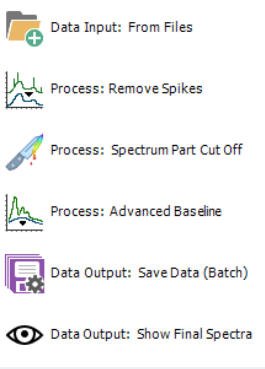
Examples:



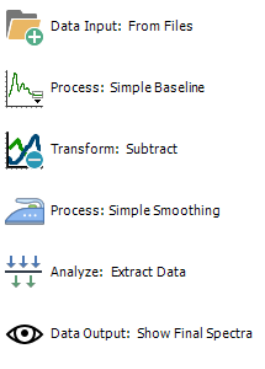
Plot creation



Batch export



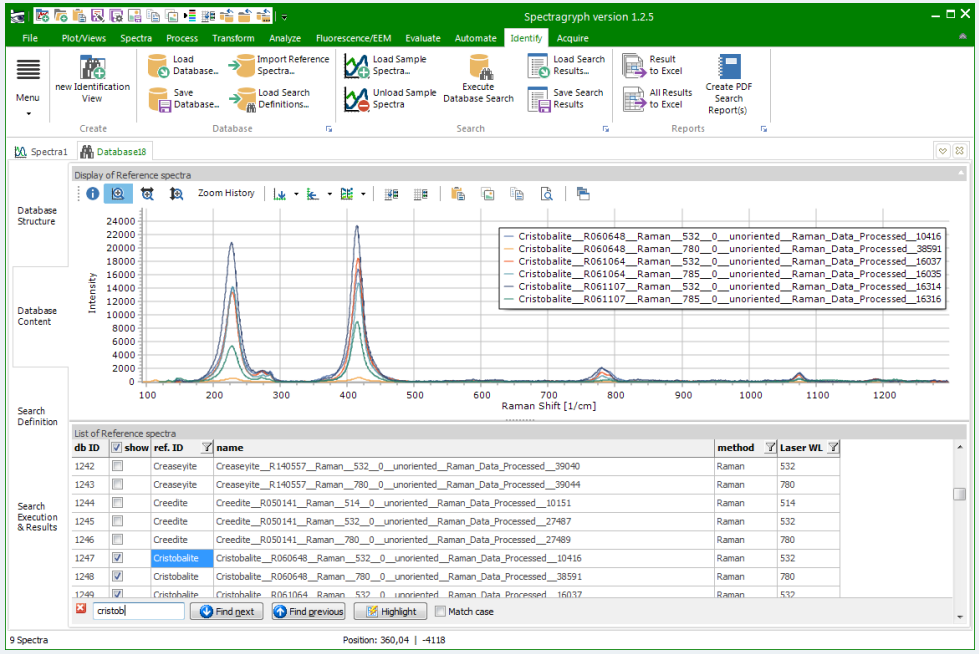
Raman processing



UV-VIS kinetics

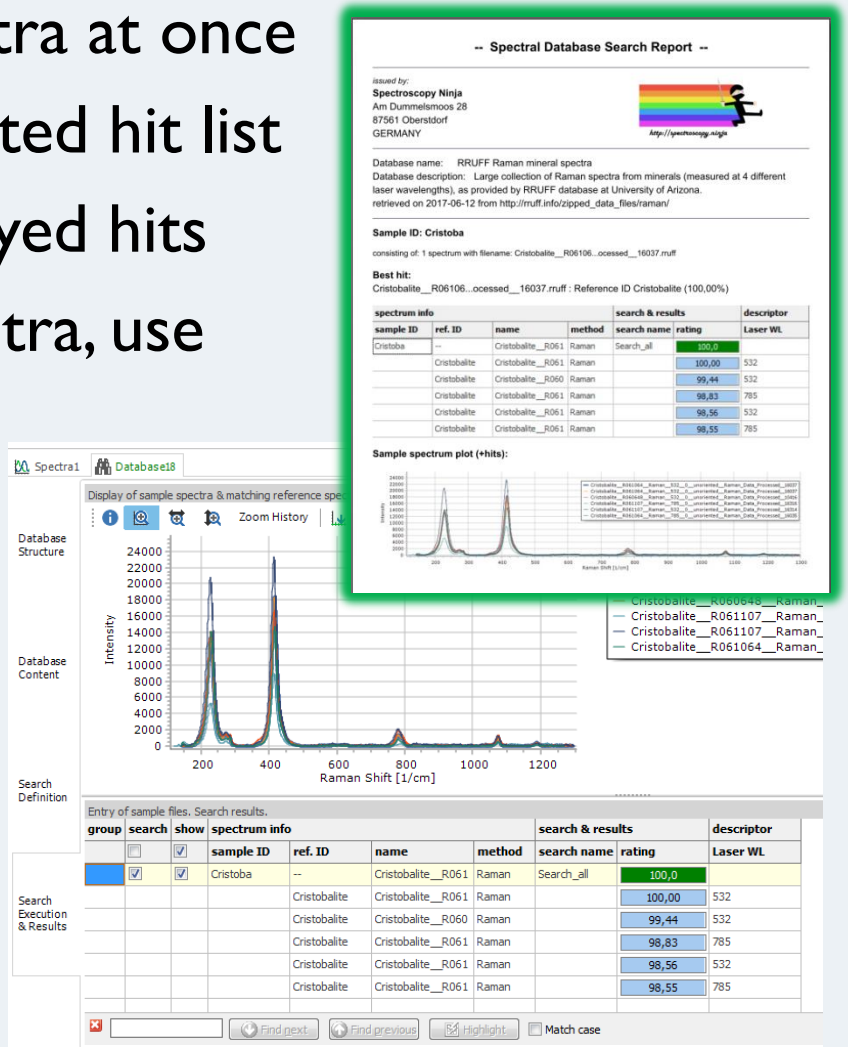
Features: Identify(database creation)

- Create custom databases from all recognized file formats
- Import commercial databases in OMNIC *.lbd/lbt format
- Define descriptors and descriptor values as meta data
- Define search & matching algorithms, combine search results with weighted hit values
- Filter searched entries by technique and descriptor values
- Multi-technique libraries, identified with sample ID



Features: Identify (search results)

- Search multiple sample spectra at once
- Display search results as sorted hit list
- Customize number of displayed hits
- Display search result as spectra, use for further processing
- Save & load previous search results
- Export results to Excel
- Create & save customizable PDF search report



Features: Acquire

- Connect to a range of spectrometers (multi-channel mode possible)
- Set acquisition parameters (exp. time, averaging, dark subtr.)
- Set acquisition mode (single shot, cont., additive, burst, loop)
- Set measurement mode (intensity, trans-mittance, reflectance, absorbance)
- X axis calibration
- Eight on-the-fly post-processing steps
- Save & load device-specific settings
- Save spectral data on-the-fly

Some Testimonials

I have started using Spectragryph since a month or so and yesterday I got myself a commercial license. It has saved me lots of time. I love the direct and friendly relationship that Dr. Menges maintains with us. He is very open to feature requests and customizing the software. Thank you Dr. Menges for Spectragryph.

Heflin Josiah Raj,
Optical Deposition Laboratory, Italy

Spectragryph is an awesome alternative to costly scientific software which only institutions can afford. Furthermore, it has just those features that are really useful for at least an audience of relatively specialized users. So, it is a great tool to disseminate spectroscopy outside of the academic applications.

Antonino Cosentino,
Director / Cultural Heritage Science Open Source
chsopensource.org

Few years ago my PhD students were using Spekwin32 software for diffuse reflectance spectra analysis of the ill and healthy skin in vivo. Recently the new students started to use for the similar scientific approaches Spectragryph software. The Spectragryph software is exceptional piece of programmer's skill and deep knowledge of spectroscopy. Spectragryph possess very sophisticated ways of different spectra analysis. It is really a masterpiece much better and flexible compare to Spekwin32 software. Dr. Menges, thank you, for your wonderful product.

Prof.Vladimir Hegyi, MD, PhD.
Institute of Clinical and Experimental Dermatovenereology, Bratislava

The Spectragryph software saved me from spending more costly hours of programming a parsing procedure for our various spectrometers. This alone was worth the cost of the software. Our Laboratory will certainly delve deeper into means of improving our procedures, analysis, and calculations with this new capability on hand. Thank you Dr. Menges, for your wonderful product. Your ninja forces are strong.

Toby S.
Research Engineer at a Polymer Testing Laboratory

"SpectraGryph is definitely going to be the Swiss-army knife for optical spectroscopy!"

"Best free software for spectral date manipulation! Must to have for researchers who do cross-instrumental comparison or love to take work home or in trip! Perfect tool for smoothing, background correction and normalization or simple visual comparison."

Peters Brangulis, Gemmologist

I think Spectragryph is an extremely user-friendly software with plenty of functions and incredible possibilities to customise your plots and numerical output. In my case, I conduct qualitative and quantitative analysis on samples of leather and synthetic polymers. I use the software to visualise spectra collected with the FTIR in my Uni lab. In the past I needed to sit in the lab to carry out the data analysis, with the constant risk of having someone interrupting to use the instrument. Now I don't need to monopolise the instrument anymore because I can do the same operations and many more in the comfort of my place. In addition, I think that the videos available online and the support provided are great. I am already promoting this software with anyone and I'll keep doing it.

Valentina P.,
University of Leeds

"Spectragryph is a great tool for teaching spectroscopy concepts in undergraduate organic chemistry. I have used it for both infrared and visible-UV spectroscopy. One especially useful feature is the ability overlay several spectra on one plot to visualize similarities and differences in the infrared spectra of classes of compounds such as alkanes, alkenes and alkynes. I have also used it with visible-UV spectra to illustrate differences in the degree of aromaticity in structurally related compounds. Students quickly grasp the menus and are able to work with the software with minimal guidance from the instructor. "

JOhn N. Rapko, Chemistry Instructor

Spectragryph is a great alternative to the proprietary and costly software that is bundled with most scientific instruments. The software offers a wide variety of display options and sophisticated methods of spectral analysis and demonstrates Dr. Menges wonderful programming capabilities and knowledge of spectroscopy. I am particularly impressed with the ability to import a wide variety of different spectral formats and am overjoyed to find that it is now also capable of searching unknown spectra against imported or custom made databases. The software is under constant development with improved versions being released on a regular basis and Dr Menges provides a quick response should you encounter any problems, so please give him your support. I am happy to recommend this software which is so useful for all types of spectroscopy and look forward to the additional features that will be incorporated into future releases.

T. Mernagh
Australian National University

Even more testimonials

"Spectragryph has helped streamline my spectroscopic analysis. The intuitive GUI makes it easy to access customization options and processing tools. I am looking forward to the future implementations of this software!"

Juan, University of Wisconsin - Madison

"I am finding more and more use for Spectragryph every day. I am amazed at how powerful the software can be and I have no hesitation in recommending it to others."

Boguslaw Szczupak
Wrocław University of Science and Technology.

"a nice software, easy to install and to use ; numerous import file format. For free researchers but still active, it is efficient and free. I use it with CrystalSleuth, and it replaces OMNIC (very expansive and large). thank you "

DAUPHIN Yannicke
ISYEB, Museum histoire Naturelle, Paris

"Spectragryph is a versatile tool, very easy to use. It allows file conversion from different instrument and therefore compare data within a range of instrument and experimenter which is more than useful during collaborative work. Therefore, it definitively made my life easier, I am not sure I would have been able to complete my work without SpectraGryph."

Helene Gaussier, Aix-Marseille University

"I was a user of Spekwin32 for some years and now Spectragryph is my workhorse for data analysis. I appreciate the huge number of file formats it is capable to read and the facility to display and analyze multiple data. Commands and shortcuts are always easy to find and use. It is really coded by a person that know about spectroscopy analysis. Thanks Friedrich for this superb software!"

Lucio Farenzena
Professor - Dep. of Physics - UFSC - Brazil

"This programme is a god-send if, like me, you have spectra from many different spectrometers to examine/ analyse. This used to be a nightmare, involving sitting at the instrument to use the in-built software, or trying to ensure propriety software copies were installed on office and home computers (not always possible, of course). I congratulate Friedrich for the professional quality of Spectragryph and hope that he can find the resources to continue supporting it. "

Prof Frank Placido
Institute of Thin Films and Sensors
University of the West of Scotland

"I use Spectragryph quite often to remove spikes from my UV-Vis spectra. These emission or excitation spectra are normally collected through an Eidinburg Instrument F920 spectrometer, which often involve many spikes due to defects of the detector or fluctuation of excitation light intensity. In Spectragryph, spikes can be easily removed and this improve the statistic quality of spectral , saving time to increase time of measuring. "

Ang Feng, PhD student, Universiteit Gent

This software is excellent for processing FTIR spectral data. I have not seen any like it yet! I was able to batch process data, to stack my spectra in ways I could not have imagined.

John Anyam, Federal University of Agriculture Makurdi, Nigeria

"Great software package. Very easy to follow, intuitive, great results, quickly! "

C. Marcelo Sergio
Garvan Institute of Medical Research

"Spectragryph is very good package for handling diverse type of spectra. It appears to be very close to some famous software dealing with spectral management. My sincere compliments to FM for an excellent job he has done. "

Zoran Matovic,
professor of chemistry/ Faculty of Science

Links

- Linkedin: http://de.linkedin.com/in/friedrichmenges
- Facebook: https://www.facebook.com/Spectroscopy.Ninja/
- Twitter: https://twitter.com/MengesFriedrich
- Youtube: https://www.youtube.com/channel/UCpjrKBe7m_Exf6-zRPIeJjw
- Website: http://Spectragryph.com
  - Features: https://www.effemm2.de/spectragryph/about_feat.html
  - User testimonials: https://www.effemm2.de/spectragryph/testimonials.html
  - Help: https://www.effemm2.de/spectragryph/about_help.html
  - Purchase: https://www.effemm2.de/spectragryph/license.html

Applications

- In heavy use by academics all over the world for
  - Conversion of original, binary file formats into something readable
  - General purpose spectral data processing for all kind of spectra from UV-VIS, NIR, FTIR, Raman, fluorescence, LIBS, XRF spectrometers
  - Freeing up instrument time by allowing researchers to treat their spectra wherever and whenever they need

  - Generating plots for posters, papers, daily work
  - Visualize, overlay and compare spectra in ways that were not possible before
  - Teaching practical spectroscopy to countless students

Special Applications I

- With the „*Automate*“ feature, take the dumb, repetitive, error-prone aspects out of spectra processing.

Example:
A user is taking 100,000s of LIBS spectra within a quantitative measurement campaign. Data reduction includes baseline subtraction, averaging, merging and peak area analysis. By putting all these steps into a Processing sequence, data reduction becomes 100% reproducible and takes only little time. No more need to save intermediate steps. Also, several calculation approaches can be easily compared from the final results. The best sequence is kept in the end and can be applied ever and ever again on arbitrary numbers of spectra.

Special Applications II

- With *Spectragryph-id-on*, and using the right spectral libraries, material identification is only two clicks away

Example:
Spectragryph-id-on controlling an Andor camera based Raman system, with the RRUFF mineral Raman database loaded into a „Identify“ tab. The little yellow fork truck carries the data from the acquisition tab to the identification tab, so it takes *only two clicks* from measurement to search result.

Watch this video:
https://youtu.be/QPYunSwUTS4

