Near Infrared Spectroscopy

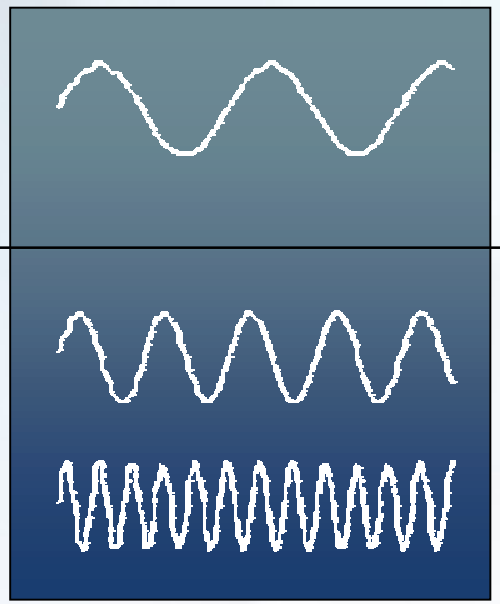
Introduction into the method

NIR Spectroscopy: Some characteristics

NIR: λ = 780 – 2500 nm (12500 – 4000 cm^{-1})

Combination and overtones of CH-, OH-, and NH- vibrations

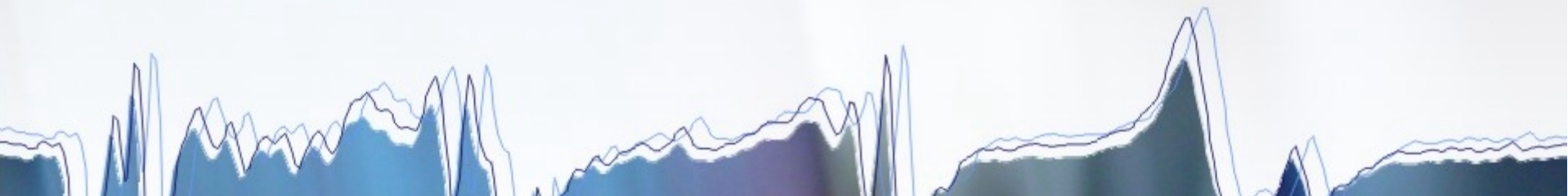
- Normal mode vibration (MIR)
- High degree of excitation



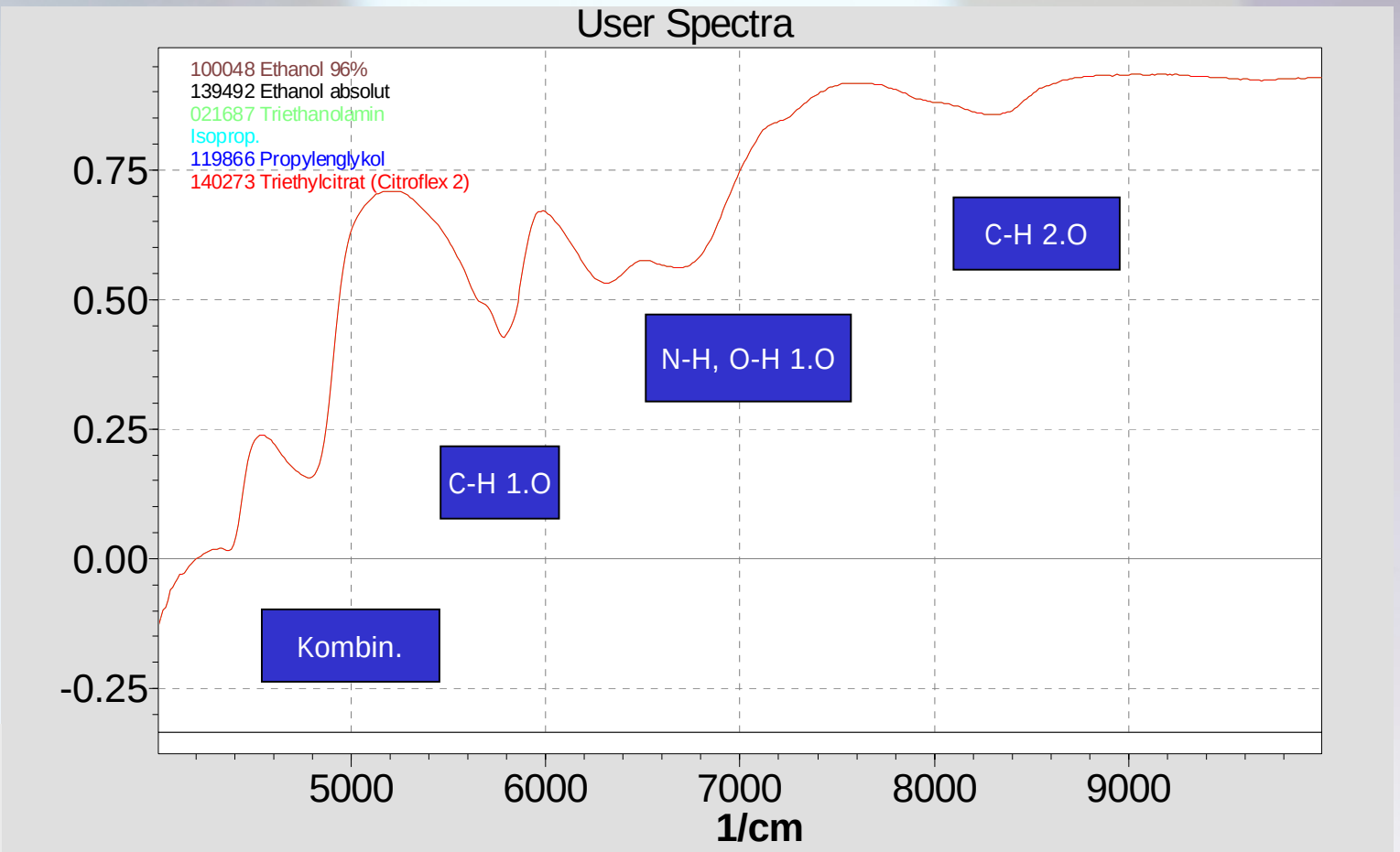
- Combination and overtones (NIR)
- Low degree of excitation

NIR Spectroscopy: Some characteristics

- In contrast to sharp absorption peaks in the MIR region, NIR spectra show less intensity and broad bands
- A assignment of peaks to individual vibrations is not possible
- Reflection intensity in the NIR region is higher than in mid infrared.



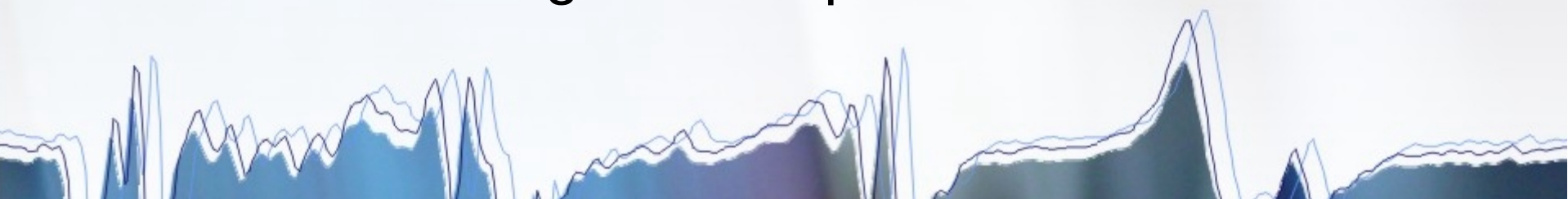
Example spectra



Advantages

- Liquids, powders and even high-viscosity substances can be measured without sample preparation
- Silica can be used as transmittance material for cuvettes, fibers and probes.
- Measurement period!

- One NIR spectra is a characteristic „fingerprint“ of an individual extract and covers all organic compounds!



Evaluation of NIR spectra

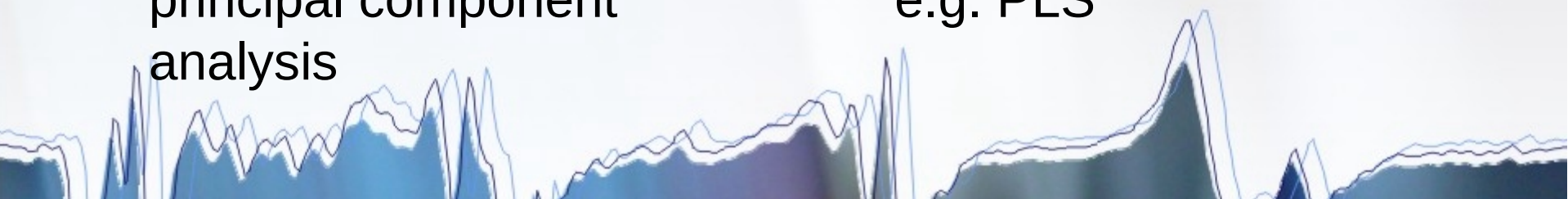
International Chemometrics Society:
Chemometrics is the science of relating measurements made on a chemi system or process to the state of the system via application of mathemat or statistical methods.

Qualitative classification

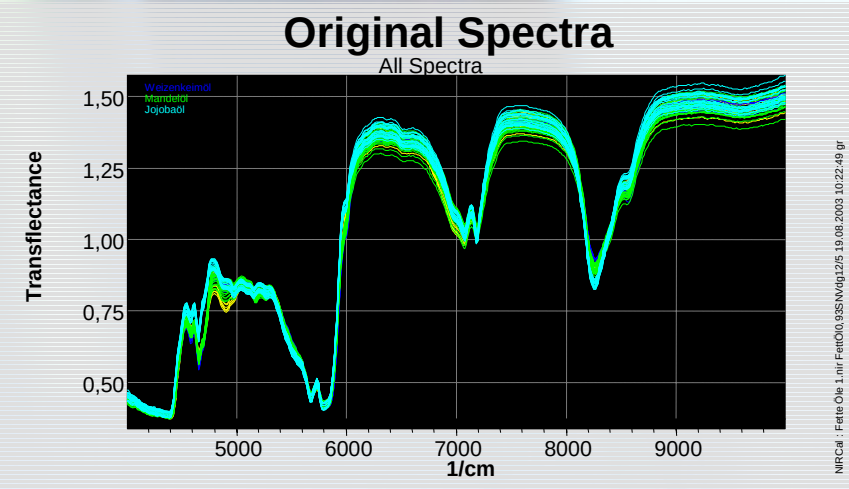
- Sufficiently big sample set with a certain variety concerning to the expected determination range
- Development of a qualitative model, e.g. principal component analysis

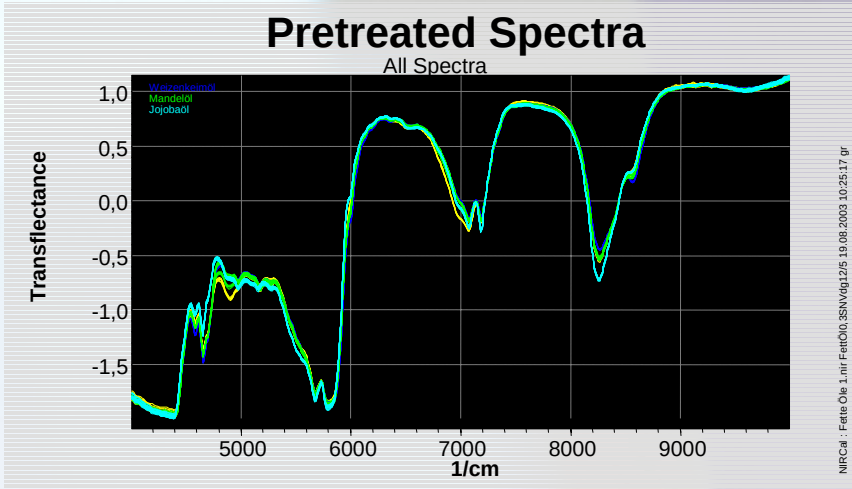
Quantitative Analysis

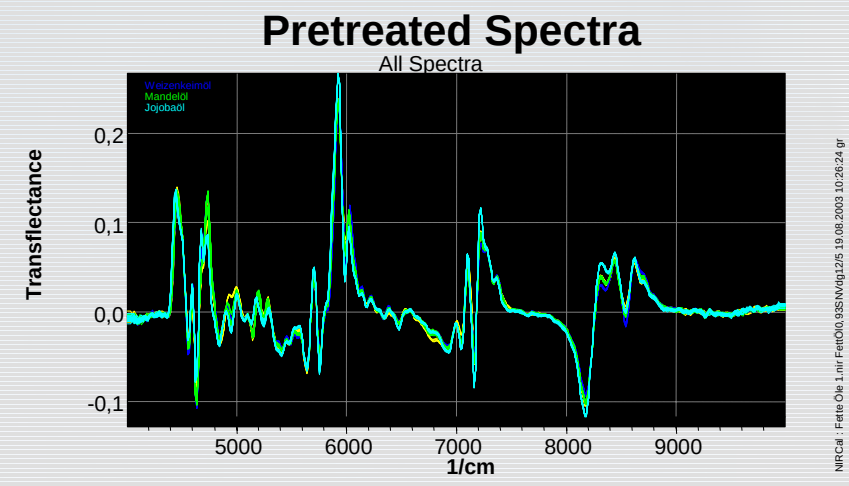
- Reference data of all samples have to be determined
- Spectral data and refernce data are combined in a calibration, e.g. PLS

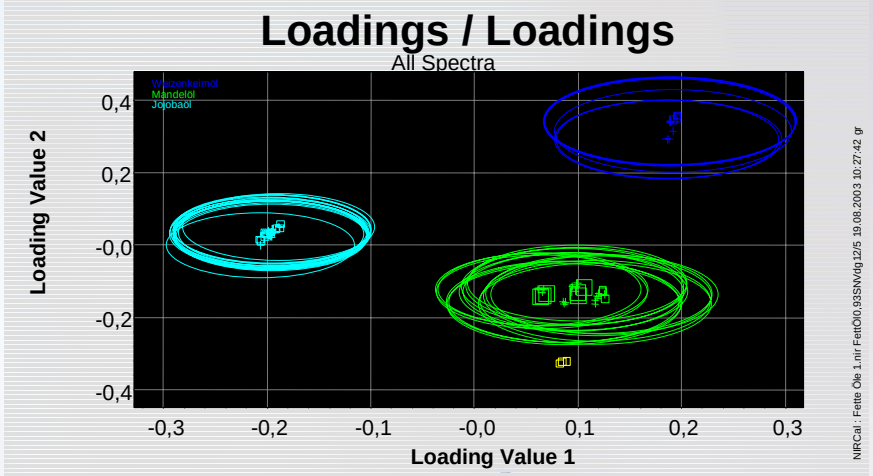


Identification procedure

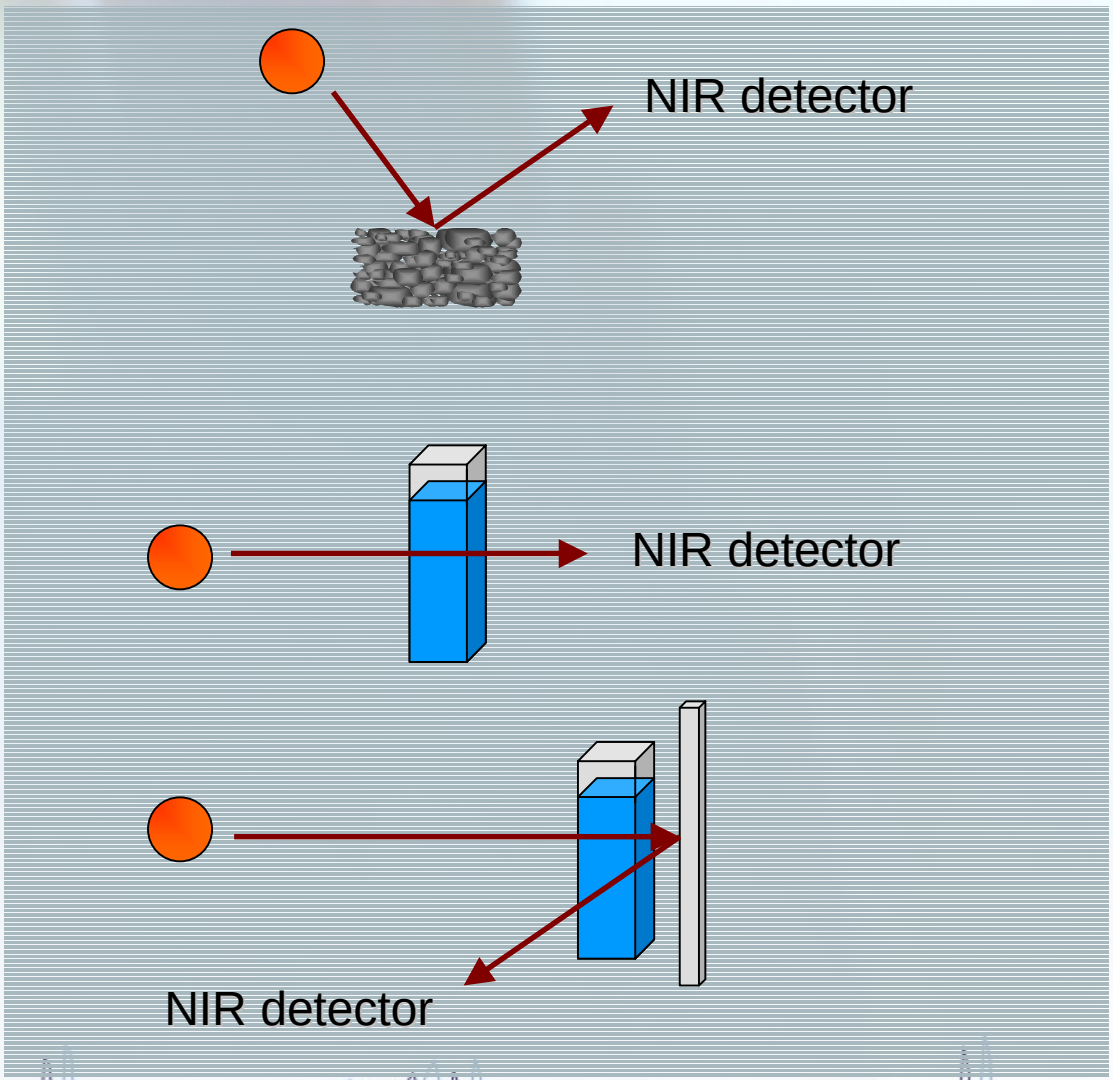








Principles for NIR measurements



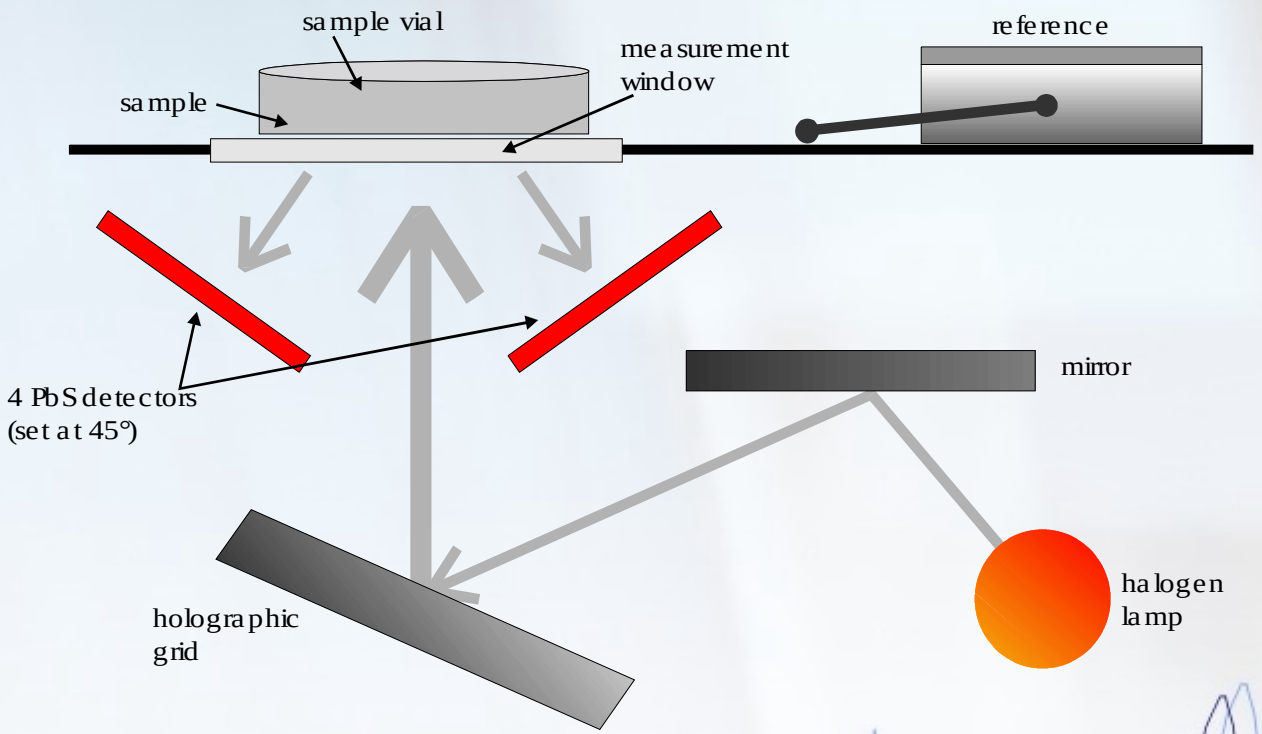
Diffuse reflection

Transmission

Transflection

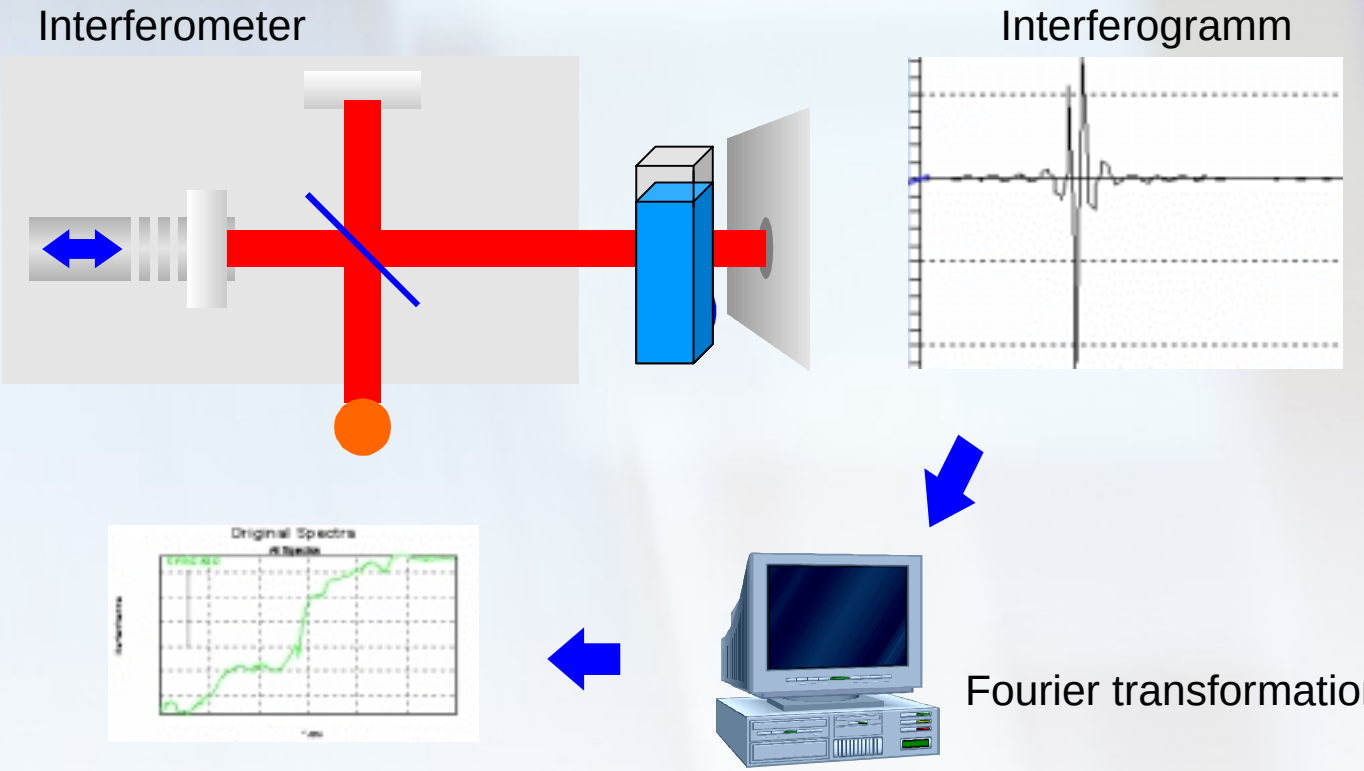
Spectrometer types

- Dispersive spectrometer (e.g. Foss NIRSystems 5000):



Spectrometer types

- Fourier transform spectrometer (e.g. Büchi NIRflex)



- Diode array spectrometer

„Interim statement“

- In NIRS single compounds influence not only individual regions, but often the whole spectrum
- Visual analysis of the spectra is impossible
- NIR spectra have no significant peaks, but they are unique „reproductions“ of a substance or a mixture
- Data have to be combined with multivariate mathematical methods

We need a different thinking, when working with NIRS !