

Development- and Quality-control for molecules of pharmaceutical interest by MID-IR and NIR Techniques.

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IR spectroscopy is a classical technique which depends upon the interaction of infrared radiation with the vibrating dipole moments of molecules. It gives, with the exception of homonuclear diatomics and noble gases, a characteristic spectrum for each substance.

FTIR Imaging:

Imaging is the favored technology for two-dimensional FTIR-Analysis with high spatial resolution. Therefore, it is very suitable for the spectral analysis of surface and thin sections. Especially for the investigation of biological materials as well as for the study of polymer blends, FTIR-imaging is a already well-established technique.

FT-NIR Spectroscopy:

The near-infrared (NIR) range of the electromagnetic spectrum extends from 800 nm to 2500 nm (12500 to 4000 cm^{-1}) and is flanked by the mid-infrared (MIR) range to longer wavelengths and the visible range (VIS) to shorter wavelengths.

While a MIR spectrum records mainly the fundamental atomic vibrations within the individual chemical bonds of most molecules, the corresponding NIR spectrum shows the so-called overtone and combination bands.

Due to the dramatic decrease in band intensity of the higher overtones, the NIR spectrum is usually dominated by overlapping overtone and combination bands of the structurally lighter groups (e.g. CH, NH and OH). In the NIR range remote measurements using quartz fiber optics are also possible and are particularly well-suited for on-line process monitoring. The attenuation of the light signal inside the fiber is very small (e.g. 0.1 dB/km). NIR fibers are robust, cheap and widely used.

NIR spectroscopy can be used for many qualitative and quantitative applications in various industries. It is the ideal technique for quality assurance (QA) or quality control (QC). QA begins with the qualitative identification of incoming raw materials and continues with on-line process monitoring. The quantitative analysis of final products is the last step of the quality control procedure.

TG-FTIR Coupling:

Thermogravimetric analysis (TG) follows changes in mass of the sample as a function of temperature and/or time. TG gives characteristic information about the composition of the measured sample, in particular the amounts of the various components and their thermal behavior.

An identification of gases released directly from the sample or during thermal treatment cannot be performed just by thermal analysis. For this purpose, coupling a spectroscopic method such as FT-IR is an excellent solution. For monitoring continuous processes, the FT technique offers the specific advantages of speed and sensitivity.