This paper describes in detail the concept of an innovative multispectral laboratory, as well as new methods for the spectral analysis of liquids, solids, and gases based on an inter spectral chemometric approach. It is intended for researchers in educational and scientific laboratories.
The multispectral laboratory concept is presented by MIR Photonics LLC, acting as a system integrator that combines spectrometers, fiber optic probes, and chemometric methods into complete analytical solutions.
The multimodal fiber optic probes used in these systems are developed and manufactured by art photonics GmbH (Berlin, Germany), a global OEM supplier of fiber optic sensing solutions covering the spectral range from UV to Mid IR. art photonics provides both standard products and customer specific probe designs, including multimodal and application tailored solutions.

Multispectral Laboratory of Optical Analysis Methods purpose, methods, and applications

Image courtesy of art photonics GmbH.

Analytical chemistry is a science that develops the theoretical basis of chemical analysis of substances and materials and develops practical methods for identifying, detecting, separating, and determining chemical elements and their compounds, as well as methods for determining the chemical composition of substances. Analysis is typically divided into quantitative and qualitative. The first answers the question, "What is the composition of a sample?", while the second answers the question, "What is its quantitative composition? How much of a particular substance does it contain?" The task of an analytical chemist is to develop and improve methods for quantitative and qualitative analysis.

This is accomplished by utilizing knowledge from various fields of science, including modern scientific and technical advances in chemistry, physics, mathematics, biology, and other fields. The analytical methods and techniques developed are aimed at solving various real-life problems: ensuring the quality of manufactured products, improving the efficiency of technological processes, protecting the environment, and medical diagnostics. Thus, analytical chemistry, like no other discipline, is directly linked to solving real-world problems. Analytical chemistry today is no longer associated with archaic, purely chemical methods such as colour reactions, precipitation, gas evolution, and combustion. Laboratory measurement methods based on titration, filtration, distillation, and weighing are becoming a thing of the past, becoming more a part of the educational process than practical chemical analysis. Modern analytical chemistry involves complex, highly automated measuring instruments that utilize a variety of effects arising from the interaction of a substance with a field, wave, or particle flow. Optical spectral analysis occupies a special place among physicochemical methods for studying substances and materials. It is based on measuring the result of the interaction of electromagnetic radiation with a sample over a wide range of wavelengths, from hard ultraviolet to far infrared light. The result of this interaction, measured using a spectrometric or sensor analyzer, carries a lot of chemical information about the analyzed object. Being extremely flexible in organizing measurements and, not requiring mandatory sample preparation, fast, and non-destructive, optical analysis is often the only alternative in solving important issues related to quality of life and safety in modern society. One of the most notable trends in the development of optical spectroscopy is the increasing use of fiber optic solutions. Fiber optic probes and cells are being integrated into reactors and production lines of ongoing technological processes, enabling on-site online analysis and obtaining results in near real time. Thanks to the achievements of photonics, optics and micromechanical engineering, the development of specialized analyzers of a new type, optical multisensor systems (OMS), is underway.

These inexpensive, compact, and portable systems are increasingly being used for field and rapid analysis. Their development is creating a new, high-tech field of analytical chemistry, which is interdisciplinary in nature and requires expertise in information technology, electronics, and instrumentation.
An integral part of modern spectral methods is the mathematical processing of complex multidimensional data to extract useful analytical information.
This is achieved through a special branch of analytical chemistry called chemometrics, which provides chemists with a rich toolkit for constructing calibration and classification models, as well as methods for in-depth research data analysis.

This paper describes in detail the concept of an innovative multispectral universal laboratory developed by ***"Mir Photonics" LLC***, — a collection of optical spectral equipment specifically selected to address a wide variety of scientific, educational, and industrial tasks. The laboratory is focused on modern analytical research, including online analysis using fiber optic cables and probes. The equipment includes spectrometers for analysis using key optical methods—ultraviolet (UV) and visible absorption, as well as near- and mid-infrared (IR) spectra, fluorescence, and Raman scattering. Measurement of a wide range of gaseous, liquid, and solid samples is organized using a variety of interfaces and enables sample analysis using transmission, diffuse reflectance, or emission measurements.
The relevant measurement and data analysis methods are provided, including software and illustrative explanations.
The facility can combine two or more spectral methods when necessary to solve particularly complex analytical problems, such as process analytical control and medical diagnostics.
The description includes typical examples of laboratory use, including the development of operational analytical methods using chemometric software.

2. Purpose of the Laboratory

The laboratory is designed to perform all major types of modern optical spectral analysis online using fiber-optic probes.
- *What is the advantage of online analysis?*
It allows for in-process analysis, i.e., directly in the process flow or reactor without sampling, eliminating delays and the risk of sample contamination.
- *What is the advantage of purchasing an entire spectral laboratory at one time, compared to purchasing it element by element?*
To answer this question, various scenarios should be considered.

2.1. Educational Use

An optical spectral laboratory designed to implement the concept of process analytical technology (PAT) through online monitoring can be used to support the educational process, for example, within undergraduate, graduate, and postgraduate programs in courses in analytical chemistry, chemical ecology, pharmaceutical and food production, and other disciplines related to chemical analysis. The use of a pre-selected, price-optimized equipment set, equipped with software and ready-made lab examples on various topics, significantly facilitates the technical organization of the educational process. Such an educational laboratory can simultaneously be used for scientific research, as shown below.

2.2. Scientific Research

An optical spectral laboratory can be used in research conducted at universities and other scientific institutions.
The exploratory nature of scientific research does not always allow for a precise prediction of which existing method will yield the desired result. The ability to test various optical spectroscopy approaches is crucial for solving complex analytical problems, such as analyzing natural and industrial samples of incompletely known composition, in order to select the most suitable method or combination of methods.

The presence of a modern, pre-designed and well-integrated laboratory of spectral analysis methods and pre-proven techniques makes it easier to obtain funded projects from the state and industrial customers.

2.3. Industrial Use

A well-thought-out combination of spectral equipment and software can significantly simplify and reduce the cost of equipping a newly established or upgraded industrial laboratory.
Industrial enterprises and commercial entities, and sometimes even scientific and educational institutions engaged in chemical spectral analysis, may lack the expertise to optimally select the necessary spectral equipment, including spectrometers, measurement interfaces, and software.
This is particularly true for the development of multispectral methods, which optimally combine two or more spectroscopy methods.
Traditionally, equipping a spectral laboratory occurs gradually, as the need for a particular analytical method and instrument arises.
This approach is often dictated by the organization's budget and allows for an even distribution of available funds. However, it is not optimal in terms of the combination of laboratory elements and does not take into account the full range of practical tasks that may arise in the future. Importantly, an integrated approach takes into account the compatibility of instruments and software, as well as the ability to work with data from various spectral formats, thereby facilitating data preparation and analysis.
Thus, acquiring an entire laboratory is often more practical than assembling it piecemeal. In addition to integrated equipment, software, and ready-made methods, a comprehensive spectral laboratory setup includes the knowledge and experience of numerous expert analysts.

3. Advantages of a Multispectral Approach

3.1. Information Capability of Spectral Methods

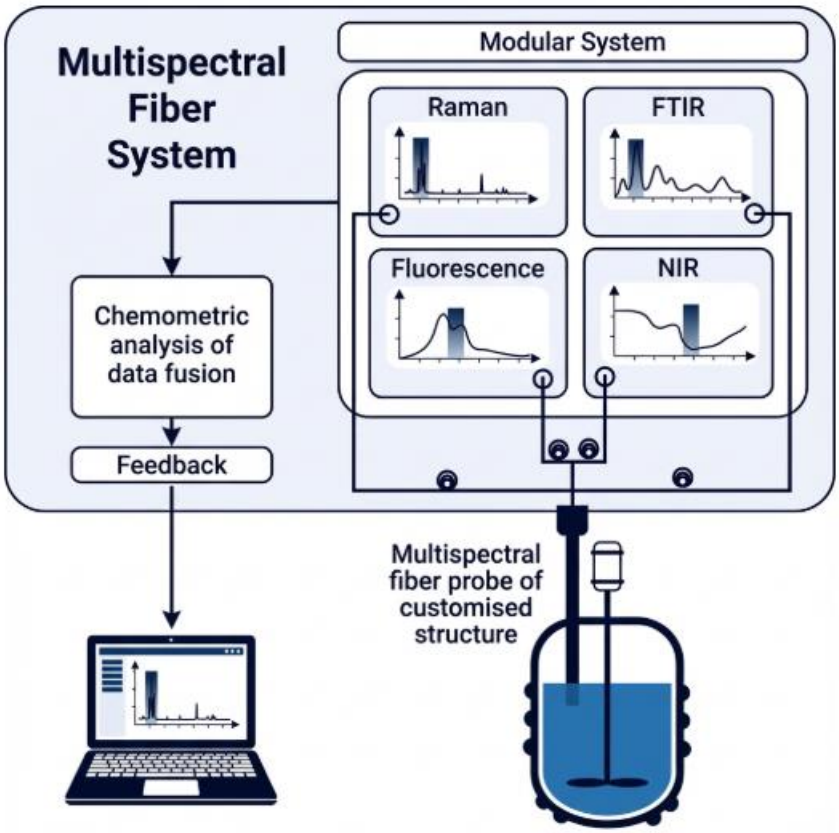
Spectral analysis provides information about the chemistry and morphology of the sample being studied: the concentrations of its components, their distribution, and particle sizes. The analytical information provided by different spectral methods can vary greatly, as it is closely related to the chemistry of the sample being studied, the nature of the physical phenomena involved, and the measurement method itself (Table 1).
One of the most informative analytical methods is molecular vibrational spectroscopy. Three spectroscopic methods are used to record energy transitions between vibrational levels of molecules: mid- or near-infrared (NIR) spectral ranges, as well as Raman spectroscopy.
Despite the theoretical similarities between these methods, their practical instrumental implementation and application in analysis differ greatly. The difference in operating wavelength ranges—from 360 nm to 25,000 nm (400 cm-1)—requires the use of different light sources, optics, and detectors, and is therefore typically implemented in separate spectral instruments. Different absorption coefficients of light in NIR, Mid-IR, and Raman spectroscopy, as well as the depth of its penetration into a given dense medium (solid, liquid, or powder) also requires different measurement interfaces and techniques, such as various fiber optic probes: ATR, Transmission, Transflexion, Reflection, etc.
These differences in methods create natural limitations for their use, meaning that a given practical analysis task requires selecting the most optimal method and approach (technique) for its solution.

For example, NIR spectroscopy, with its relatively large penetration depth (up to several millimetres) even into dense solid samples due to low absorption and strong scattering, allows the use of ordinary glass for optics, as well as standard lamps as light sources, making it ideal for online applications, including remote measurements via fiber optic probes. In contrast, strong absorption in the mid-IR region limits the corresponding spectral method to the analysis of very thin samples (usually less than 50 μm), but it opens up the possibility of using attenuated total reflectance (ATR) by connecting appropriate attachments and probes.
Measurement of the weak Raman effect requires special probes but is recorded in the visible and NIR spectral regions. Moreover, the spectra of vibrational transitions in Raman and mid-IR spectroscopy carry complementary qualitative and quantitative information about the sample's composition.
UV-visible spectroscopy is based on electronic transitions between molecular energy levels. It has very high sensitivity, especially in the UV region (190-360 nm), but requires the use of special light sources and fiber optic probes. However, the strong overlap of spectral signals in UV spectra complicates the analysis of real samples and makes the use of chemometric algorithms a necessary component of qualitative mixture analysis methods. Another highly sensitive method, UV/Vis fluorimetry, is based on the secondary emission of excited molecules of certain substances, most often of biological origin. However, most chemicals do not exhibit this property.
Therefore, fluorimetry is primarily used in medicine, biology, and biotechnology.
Spectra from different methods vary greatly, both in their nature and in the information they contain. Mid-IR band spectra contain well-defined peaks (absorption bands), while NIR, UV, and fluorescence spectra contain broad, highly overlapping signals, forming a so-called continuous spectrum.
Extracting the information necessary for quantitative and qualitative analysis from optical spectra requires special methods for analyzing multidimensional data, called the above-mentioned term chemometrics. Chemometric algorithms are implemented in specialized software that enables preliminary data preparation (preprocessing), construction, validation, and application of predictive models, specifically calibration or classification models.
Immersible fiber optic probes operating in various spectral regions from UV to mid-IR are increasingly being used for measuring liquid and soft or powdered solid samples. They can be used to obtain absorption, diffuse reflectance or transmission, Raman, and ATR spectra. The use of these probes can be essential for in-situ analysis—in the field or in an ongoing process. Online measurements require high-speed spectral acquisition.
Often, analytical results must be obtained in real time to be used for management decisions.
An analysis of individual spectral methods, their capabilities, and limitations, demonstrates that developing an optimal instrumental methodology for solving a given analytical problem requires considering many different factors. Thus, selecting a spectral method for a specific analytical problem is a complex task requiring specialized knowledge in chemistry, physics, and mathematics. This is especially true for equipping an entire laboratory for future needs, since the need for a particular optical analysis method is difficult to predict in advance. In the equipment package offered here, called a multispectral laboratory, experts from various fields have already worked hard to select the optimal solutions.

Table 1. Comparative characteristics of spectral methods and measurement techniques.

№	Method	Measurement method	Physical phenomenon	Sample Type	Optical path, depth	Sensitivity	Selectivity	Cost
1	**IR spectroscopy**	ATR- platform	absorption	liquid,paste, soft	1-6 mu	average	high	high
		ATR probe*						
		cuvette		liquid	10-100 mu	high		average
		sample layer		solid film	5-50 mu			
		sample surface	diffuse reflection	solid	10 mu	average		
2	**NIR spectroscopy**	cuvette	transmission	liquid	1-5 mm	average	average	average
		Transmission or transflection probe		liquid, colloidal	1-10 mm			average
		Diffuse reflection-probe	diffuse reflection	Scattering media, powder	0.5-1 mm			
		integrating sphere		solid, powder	5-10 mm			
		surface at a distance		solid, powder	2-5 mm			average
3	**Raman spectroscopy**	cuvette 90°	raman scattering (emission)	liquid	2-5 mm	average	high	high
		Raman-probe		liquid, powder, solid				
4	**UV/Visible spectroscopy**	cuvette	absorption	liquid	1-5 mm	high	low	low
		ATR probe			0.1-1 mu	low		average
		Diffuse reflection-probe	diffuse reflection	solid, pill	1-5 mm	low	low	low
		Transmission or transflection probe	Transmission	liquid	1-10 mm	low		
		probe, lens	emission of an external source	radiating sample	any	high		
5	**Fluorimetry**	cuvette 90°	fluorescence (emission)	liquid	10mm	high	low	low
		fluorimetric probe		liquid, solid	1-5 mm			

3.2. Synergy of Combining Spectral Methods



The information provided by a particular optical spectral method may be insufficient when analyzing real samples. These include complex multicomponent mixtures, most often of natural origin, such as oil, milk, process media, fermentation media, and biological tissue. Analysis of such samples is often complicated by the overlap of several phenomena: absorption, Rayleigh and Raman scattering, and fluorescence. Morphological factors, such as sample inhomogeneity (e.g., biological tissue) or process turbulence, must also be considered when selecting a measurement technique. The analysis of such systems may require a combination of two or even more spectral methods. This often provides a synergistic effect, allowing one to solve a problem that either method alone cannot handle or only partially. Thus, the combination of NIR spectroscopy with fluorescence spectroscopy demonstrated the possibility of more accurately determining the biomass content during yeast fermentation, as well as distinguishing between their intra- and extracellular metabolites.

The combination of NIR and IR spectroscopy showed benefits in determining tumor boundaries in medical diagnostics. The combination of fluorescence and IR spectroscopy also proved necessary for classifying biological tissues. Online analysis of the pellet coating process in a fluidized bed showed the best results with the simultaneous use of NIR and Raman spectroscopy. There are many other examples of the successful combination of various spectral methods in the problems of quantitative determination or classification of objects. This approach is called multispectral optical analysis, and it is finding increasing application in practice. The basis of the synergetic effect observed when using these two or more methods is the combination of heterogeneous information about the object. This may be chemical information of various kinds, such as in the combination of complementary

vibrational IR and Raman spectra of molecules. It may also be morphological information about the sizes of scattering particles, as in milk analysis. Information can also be obtained from various depths, as in the analysis of biological tissue samples using Mid-IR and NIR spectroscopy with fiber-optic probes.

3.3. Obtaining and analyzing multispectral data

To maximize the benefits of a multispectral approach, it is necessary to properly collect and analyze the obtained data, which can be quite diverse in properties, form, and content. Specialized measurement interfaces, such as probes, have been and continue to be developed for collecting multispectral data, and special chemometric algorithms are being developed for their effective analysis. The main challenges of multispectral analysis and their solutions are presented below.

3.3.1 Simultaneous Measurement by Two or More Spectral Methods

Analysis of solid, inhomogeneous samples, such as biological tissue, is often performed using fiber-optic probes. It is crucial that the spectral information obtained by different methods—Mid-IR, NIR, Raman, and fluorescence spectra—is collected from the same small, even pinpoint, area of the sample. This is difficult to achieve by using two probes alternately for measurements. High accuracy can be achieved by using specially developed multispectral probes. One such probe, optionally supplied with the multispectral laboratory, allows for the combination of Mid-IR spectral measurements using the ATR method with fluorescence and even Raman spectra. Additional measurements are performed through an ATR zirconium oxide crystal, shaped like a truncated cone. For this purpose, an additional pair of silica fibers transmitting in the UV and visible regions is connected to the base of the crystal. Another multispectral probe is also under development, combining four spectral methods: Mid-IR, NIR, Raman, and fluorescence. The problem of simultaneous measurements also arises in the multispectral study of fast processes. In this case, two or more probes, belonging to different methods, can be used for measurements, but the data from each method must be obtained simultaneously. The use of a combined probe facilitates measurements and allows for the analysis of a smaller sample volume. Situations are also possible where problems of inhomogeneity and rapid changes in the sample coexist. In these cases, the use of multispectral probes becomes essential.

3.3.2 Features of Multispectral Data Analysis

When analyzing processes simultaneously using different methods, data synchronization can be challenging, as the acquisition rates of different spectra can vary greatly—from milliseconds to minutes, while the interval between measurements can also differ. Ultimately, the measurement data must be normalized to a common time step. Successful synchronization of methods is achieved primarily by properly selecting the spectral acquisition conditions. Since perfect synchronization is often difficult to achieve, post-synchronization of measurements is usually required by selecting the optimal time step and selecting suitable data, as well as processing them, such as averaging. This function must be performed by data processing software algorithms. After data from different methods is synchronized and combined into a single matrix, it is not always possible to use the combined data "as is." Variables obtained from different spectral methods are not equivalent. If the variables have different units of measurement, the data should be normalized in some way, for example, using an autoscaling algorithm. However, normalization may not resolve all problems. Thus, the variables of

different methods can vary greatly in quality. That is, one part of the data matrix may contain more useful information (higher variance) than another. Variables of different methods may differ in the level of noise or irrelevant variance they contain. Furthermore, methods containing a larger number of variables have a greater impact on the model. To effectively analyze multispectral data, avoiding the above-mentioned problems and maximizing the benefits of combining spectral methods, specialized data fusion algorithms are being developed.

3.3.3 Instrumentation for Multispectral Analysis

One of the challenges of multispectral analysis is the need to simultaneously connect at least two independently operating measuring instruments. These are often benchtop laboratory spectrometers, which take up considerable space. Each spectrometer is typically connected to a separate personal computer or laptop. The cost of such spectrometers is also quite high. There is only one way to move away from cumbersome and expensive solutions in multispectral analysis. The development of specialized analyzers—optical multisensor systems (OMS)—focused on a specific analytical task is necessary. The growing use of OMS is a trend in the development of analytical chemistry. The next section is devoted to the use of a multispectral laboratory in the development of OMS.

4. Multispectral Laboratory in the Development of Optical Multisensor Systems

The development of OMS begins with in-depth studies of the analyzed object using standard laboratory spectrometers. This is necessary to calculate the optimal configuration of the future multispectral analyzer, for example, the optimal spectral ranges for analysis to select the necessary elements—LEDs, filters, etc. It is important to understand that, unlike classical spectral methods such as UV and visible, NIR, and mid-IR spectroscopy, OMS are not limited to the same spectral ranges. For example, LED analyzers can simultaneously contain radiation sources from any of the above-mentioned regions. An ordinary blue LED with a wavelength of 400 nm can be adjacent to an LED in the near-IR region, having an intensity maximum at 1940 nm, and even to an LED in the mid-IR range, for example, 3 μm (about 3300 cm-1). Moreover, the combination of several spectral regions at once does not lead to significant complexity of the design. Here are just a few examples of LED OMS that are the most common and practical:

- a probe for determining tumor boundaries in kidney cancer and rectal cancer;
- an RGB sensor for determining fat and protein in cow's milk;
- an LED probe moisture analyzer for bulk materials.

5. Hardware and Software

5.1. Mid-IR Spectrometry (includes FTIR Mid-IR spectrometer, ATR fiber probe)

Vibrational spectroscopy in the mid-IR range (4000–400 cm-1) is one of the most informative methods of chemical analysis. Due to the high extinction coefficients of various molecules in this region, the method is highly sensitive and can be used to analyze a wide variety of samples: solids, liquids, and gases.

ATR fiber probes (Fig.1) enable the analysis of liquids and solid elastic samples, such as biological tissue, using specialized probes utilizing high-transmission fiber optics in the Mid-IR region.
These immersion probes operate on the ATR principle but allow analysis at a significant distance from the spectrometer, without the need for sampling. Probe-based analysis is gaining widespread use in online analysis, such as in-line, in-process (chemical, biotechnological, natural) environments, as well as in-situ measurements, such as for field testing or for spectral diagnostics during surgery.

Fig.1 ATR fiber probe. *Images courtesy of art photonics GmbH.*

5.2. Near-IR Spectrometry (includes FTIR, NIR-IR, or diffraction grating/slit spectrometer, Diffuse Reflection fiber probe, or Transmission fiber probe)

Near-IR vibrational spectroscopy (NIR) is the most common online analysis method performed using fiber optic probes. NIR spectra (780–2500 nm) contain predominantly overtones and component bands of fundamental vibrations of molecules and atomic groups, such as -OH, -NH2=NH, -CH3, =CH2, ≥CH, etc., found in many organic and inorganic compounds. Unlike mid- IR spectroscopy, measurements in the NIR region are facilitated by a number of factors: the transparency of plain and quartz glass (which allows the use of standard optics and probes), low molar absorption coefficients, and high light scattering by solid and dispersed samples, which enables measurements using diffuse reflectance, including measurements without direct contact with the sample, at a distance. The broad absorption bands observed in this region overlap, suggesting the use of chemometrics for quantitative and qualitative analysis of spectral data. In terms of instrumentation, the kit can include both FTIR spectrometers (based on a Michelson interferometer), which provide high accuracy and resolution, and more affordable high-speed analyzers based on diode arrays (DADs). DDA detectors are arrays of photodiodes that allow instantaneous recording of light intensity at all wavelengths simultaneously, which is critical for monitoring fast processes.

Fig.2.1 NIR Transflexion fiber probe

Fig.2.2 Mid-IR Transflexion fiber probe

Images courtesy of art photonics GmbH.

5.3. Raman Spectroscopy (The kit includes a Raman spectrometer, laser, and Raman fiber probe.)

Measurement of the Raman scattering (RS) effect, is also a type of vibrational spectroscopy. Raman spectroscopy is based on recording weak radiation signals observed when a sample is irradiated by a laser or high-power LED, typically in the visible light range. Some of these signals are observed with a shift toward longer wavelengths compared to the excitation wavelength (Stokes shift). The difference between the observed frequencies and the laser frequency is called the Raman shift, expressed in units of frequency–wavenumbers (cm-1). The Raman shift is used as the horizontal (spectral) axis in Raman spectroscopy, while the vertical axis shows the absolute intensity of the recorded signals (photon counts). Because Raman spectroscopy reflects energy transitions between vibrational levels of molecules and groups of atoms, peaks of the same fundamental frequencies in IR and Raman spectra are located at the same positions on the wavenumber scale. However, their intensities can differ significantly, to the point that some bands may not appear in one of the spectra (symmetry prohibition). This property makes mid-IR and Raman spectra complementary, that is, they complement each other. Therefore, using these methods in tandem provides more structural information about the molecules being studied than either method alone. From a technical standpoint, measuring Raman spectra is hampered by the low intensity of Raman signals, which are several orders of magnitude weaker than IR absorption peaks in the IR range (when these spectra are compared in the original photon count units). Furthermore, observing Raman bands is often complicated by light scattering from the illuminating laser, and for many organic compounds, by the superposition of luminescence (fluorescence), which has a significantly higher intensity. These effects can be eliminated by using specialized optical filters and probes of a special design. The Raman spectrometer detector must be highly sensitive and have a wide dynamic range. Because of these characteristics, a Raman spectrometer has significant design differences from a spectrometer for recording absorption spectra, which operates in the same spectral region (400–1100 nm) of visible and shortwave NIR radiation.

The Raman spectrometer supplied with this multispectral laboratory is designed to record Raman spectra of various samples, such as liquid mixtures containing organic and inorganic substances, biological tissue, powdered materials of various origins, etc. The resulting spectra can be used for both qualitative and quantitative analysis of mixtures. Measuring the IR and Raman spectra of the same sample can be helpful in interpreting complex organic molecules. The Raman signal's

dependence on concentration is linear over a wide range of intensities. Therefore, Raman spectra (as well as IR absorption spectra) can be used to construct chemometric models—calibration or classification ones.

Fig.3 Raman fiber probe. *Images courtesy of art photonics GmbH.*

5.4. Fluorescence Analysis (includes a fluorescence spectrometer, excitation laser, and fluorescence fiber probe)

Fluorimetry is based on measuring the broad emission signal observed upon irradiation of certain samples in the UV and visible regions. The fluorescence peak is shifted to longer wavelengths compared to the excitation radiation of the source (laser or LED). This method is frequently used in biology and biotechnology. Recently, it has become a key method for online analysis of biotechnological processes. Fluorescence spectroscopy can be used for multispectral measurements, for example, in combination with Mid-IR or NIR spectroscopy.

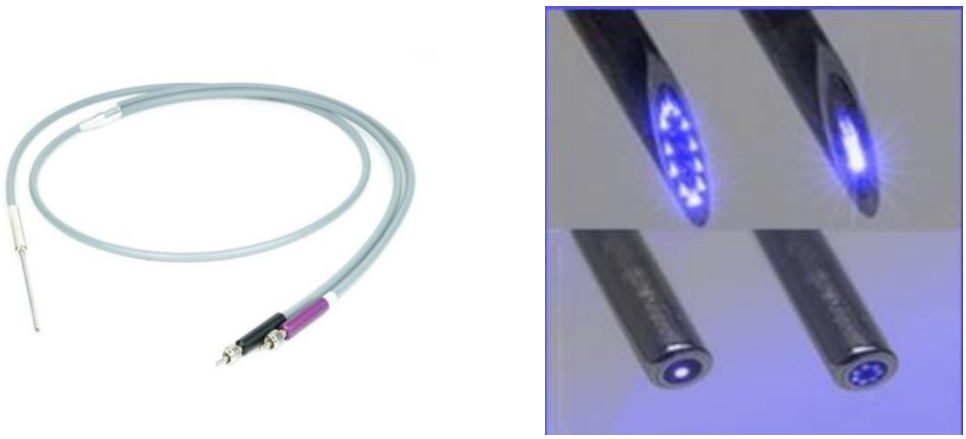


Fig.4 Fluorescent fiber probe. *Image courtesy of art photonics GmbH.*

Application cases for multispectral labs.

Multispectral labs utilizing combined fiber optic spectroscopic techniques, such as Mid-Infrared (MIR), Raman, Near-Infrared (NIR), and fluorescence, are designed to solve complex analytical challenges by providing complementary information from the analyzed media simultaneously. Below are descriptions of tasks, cases and potential applications where such multispectral systems and labs are extremely valuable.

1. Medical Diagnostics - Tumor Margin Recognition and Tissue Classification

The primary objective of this task is to provide real-time, high-precision identification of diseased tissues and the exact boundaries of tumors during surgical interventions. By accurately distinguishing between normal and malignant cells, surgeons can ensure the complete removal of cancerous tissue while preserving as much healthy organ structure as possible. This multispectral approach addresses the challenges posed by the inherent heterogeneity of biological tissues, which often makes it difficult to rely on a single spectroscopic method for a definitive diagnosis.

To perform this task, the multispectral laboratory can utilize an advanced analytical platform consisting of a combination of various spectral system such as

- High-resolution FTIR spectrometer for mid-infrared (MIR) analysis together with mid-infrared ATR probe
- UV-VIS spectrometer and 470 nm laser coupled with a fluorescence fiber probe
- NIR spectrometer and NIR light source (Tungsten-Halogen Lamp) coupled with a NIR reflection fiber probe

The experimental procedure involves the direct contact of the probe tip with the tissue during an operation, such as for kidney, colon, or rectal cancer. The MIR-ATR component captures the "chemical fingerprint" of the tissue's surface layer, typically at a depth of few microns, providing information on molecular composition and biochemical changes. Concurrently, the fluorescence or near-infrared (NIR) signals penetrate deeper into the sample, offering morphological insights and subsurface chemical data. This simultaneous measurement is crucial for medical applications where local tissue properties and precisely localized data are required to make surgical decisions.

The data processing is organized through a multi-step chemometric workflow with data fusion to create a unified matrix. Advanced algorithms, such as Principal Component Analysis (PCA) or Partial Least Squares Discriminant Analysis (PLS-DA), are used to validate and run classification models. These models automatically categorize the tissue as "normal" or "malignant," providing instant diagnostic results that serve as a "spectral biopsy".

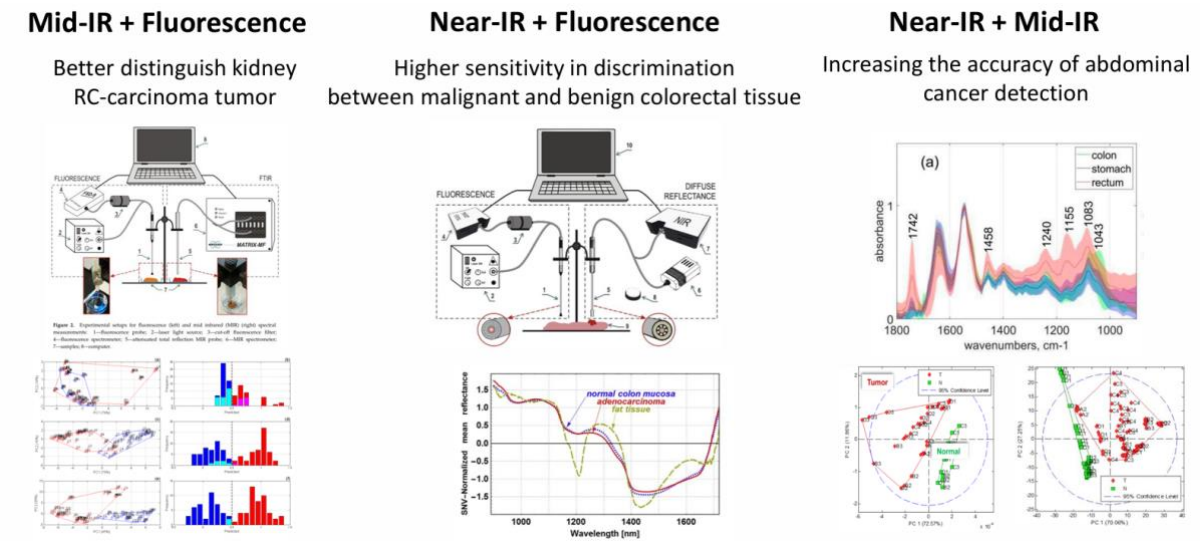


Fig. 5. Multispectral approach examples in differentiation between healthy and tumor tissues.
Image courtesy of art photonics GmbH.

A multispectral fiber probe, e.g. one combining MIR-ATR and fluorescence techniques into a single fiber optic probe shaft allows for the simultaneous acquisition of complementary chemical information from the exact same measurement point, a capability critical for analyzing heterogeneous solid samples like biological tissues or rapidly changing liquid environments.

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2. Pharmaceutical Manufacturing - In-line Monitoring of Blend Potency and Coating Processes

A multispectral lab can be also focused on ensuring the quality and consistency of pharmaceutical products through in-line monitoring of critical manufacturing stages, such as powder blending and pellet coating. The primary objective is to determine "blend potency" - the precise concentration and uniformity of the Active Pharmaceutical Ingredient (API) - directly within the production line, specifically in the feed frame of a rotary tablet press. In the pharmaceutical industry, the most popular

and widely implemented spectral techniques are Near-Infrared (NIR) and Raman spectroscopy. The combination of these techniques is particularly effective because it captures complementary chemical information: NIR detects hydrogen bonds and asymmetric polar groups, while Raman provides information on the molecular backbone and symmetrical non-polar groups.

The equipment used for such task involves next spectral systems:

- NIR spectrometer and light source coupled with a NIR reflection probe
- Raman spectrometer and Raman fiber probe for contact measurements with 785 nm excitation wavelength

During the experimental action, the probes are inserted directly into the process environment, such as the feed frame of a rotary tablet press. As the powder blend passes the probe tip, the system captures spectra at high speeds without interrupting the production flow. This setup allows the laboratory to track dynamic changes, such as the gradual increase in coating thickness or the homogenization of a multi-component blend, in real-time. The use of fiber optics is critical here, as it allows the sensitive spectrometers to be located safely away from the vibration and dust of the manufacturing floor.

Data processing for pharmaceutical tasks relies on "low-level data fusion," where the synchronized NIR and Raman spectra are merged into a single augmented matrix. Then regression models, such as Partial Least Squares (PLS), are applied to these fused datasets. By combining Raman and NIR, these models can predict API potency or coating thickness with higher accuracy and robustness than single-method models.

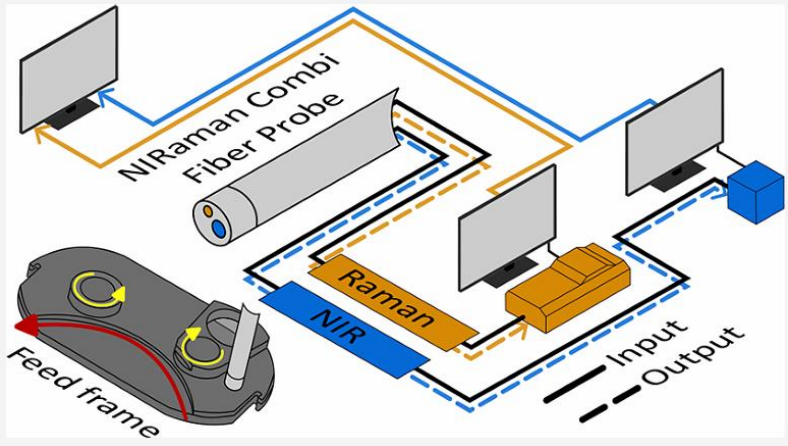

Fig. 6. A multispectral NIRaman fiber probe has industrial grade design that combines NIR reflection and Raman optical techniques in a compact shaft that fits in a tablet press feed frame.

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3. Fiber Optic Techniques for Real-Time Monitoring of Bioprocessing.

Having access to a full suite of fiber-optic spectroscopic techniques - rather than relying on a single method - allows a lab to address the diverse analytical challenges of bioprocessing, where no single sensor is universally optimal for every analyte or condition. Each technique offers distinct advantages in sensitivity, specificity, and cost-effectiveness that can be strategically combined to optimize production.

- **Multimodal Metabolite and Biomass Tracking**: a primary advantage of having multiple techniques is the ability to monitor both complex chemical structures and overall physical process trends simultaneously. For instance, UV/Vis spectroscopy can be deployed as a low-cost, robust tool for real-time biomass monitoring, as cell suspension turbidity correlates well with cell density. While UV/Vis tracks growth, Raman spectroscopy can be used in the same reactor to provide a "molecular fingerprint" for direct detection of specific metabolites like glucose, acetate, or lactate. This combination is practical because Raman is particularly well-suited for aqueous environments, as it exhibits low absorbance for water molecules compared to infrared methods.

- **Precision Monitoring Across Concentration Ranges**: labs equipped with both Near-Infrared (NIR) and Fluorescence spectroscopy can solve the problem of monitoring analytes at widely varying concentrations. NIR spectroscopy is effective for tracking major components like glucose or glycerol in the millimolar range but may lack the sensitivity to detect trace compounds below 0.1 percent. To fill this gap, Fluorescence spectroscopy can be used for high-sensitivity detection (down to the nM-µM range) of critical cofactors and amino acids like NADH, tryptophan, and riboflavin. By using both, a researcher can maintain high-precision control over both the main carbon source and the delicate metabolic state of the cells.

- **Precision Monitoring Across Optical Density Ranges**: When measuring media in the UV-Vis spectrum, the selection of an optical probe is primarily dictated by the sample's optical density (OD) and its ability to attenuate light. For highly transparent liquids with low optical density, UV-Transmission or Transflection probes are ideal; they pass light through a defined path length (typically 1 mm to 10 mm), allowing for high sensitivity and accurate quantification of low-concentration analytes. However, as the media becomes more opaque, turbid, or highly concentrated, the signal in a standard transmission setup becomes saturated because the light cannot penetrate the bulk of the sample. In these high-OD scenarios, a UV-ATR (Attenuated Total Reflection) probe is used. Instead of passing light through the sample, ATR relies on the evanescent wave that penetrates only a few micrometers into the medium at the crystal interface, effectively creating an extremely short path length that enables the measurement of "black" or highly scattering fluids without dilution.

Equipping a facility with both probe types significantly increases laboratory flexibility, as it allows researchers to pivot between different samples without changing instruments. This versatile analytical capability enables the lab to participate in a broader range of research projects, spanning from traditional pharmaceutical quality control to the complex monitoring required in advanced materials science and industrial process development.

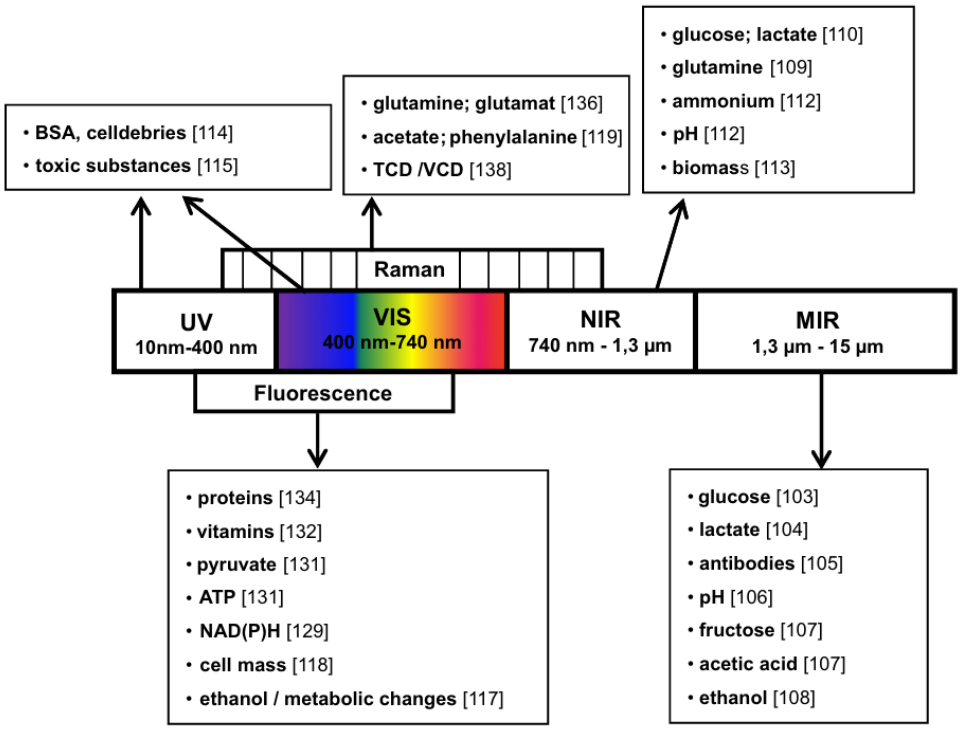

Fig. 7. Spectral range for bioprocess monitoring with accessible variables.

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- Mishra, A., et al. (2025). Spectroscopic advances in real time monitoring of pharmaceutical bioprocesses: A review of vibrational and fluorescence techniques. *Spectroscopy Journal*, *3*(2), 12.

4. Inline Milk Analysis.

The use of Near-Infrared (NIR) spectroscopy for the inline monitoring of milk is a cornerstone of modern dairy "Process Analytical Technology" (PAT). Maintaining both **NIR Reflection** and **NIR Transmission** techniques in a lab environment provides a comprehensive analytical suite capable of handling the diverse physical properties of dairy products.

- **NIR Reflection:** Inline NIR Reflection is primarily used for opaque or highly concentrated dairy products, such as yogurt, butter, or whole milk concentrates. The main equipment includes a fiber optic probe where one set of fibers delivers light to the sample and the other collects the "backscattered" light. Experimentally, the probe is flush-mounted into a pipe or vat to interact directly with the flowing medium. Because the light does not penetrate deeply, the method is sensitive to the surface characteristics and fat globule size. Data processing may involve converting the reflectance values to absorbance and applying Multiplicative Scatter Correction (MSC) or Standard Normal Variate (SNV) transformations to remove physical interference caused by the scattering nature of the milk particles before using Partial Least Squares (PLS) regression to quantify fat and protein.

- **NIR Transmission:** NIR Transmission is the preferred method for transparent or semi-transparent liquids, such as skim milk, whey, or permeate. The setup typically consists of a transmission / transflection probe, where light passes entirely through a defined layer of the sample to a detector on the opposite side. The key experimental action is the precise control of the optical pathlength (usually 1 - 10 mm); if the pathlength is too wide, the signal is lost to absorption; if too narrow, the sample represents a negligible volume. Data processing focuses on the Beer-Lambert law, where the measured transmittance is converted to Absorbance. This technique generally offers higher accuracy for low-concentration components because the light interacts with the entire volume of the sampled cross-section, providing a more representative chemical signature.

- **The Advantage of Dual-Technique Availability:** having both fiber optic techniques available in a lab rather than relying on one provides the flexibility needed to monitor the entire production chain. While transmission is superior for the high-precision analysis of dilute process streams (like whey filtration), it fails when the milk becomes too "thick" or fat-rich, as the light cannot penetrate the sample. Conversely, reflection can work well in highly scattering environments but can be less representative for clear liquids. By maintaining both, a lab can calibrate models for every stage of production - from raw milk intake to final evaporation - ensuring that no matter how the physical state of the milk changes during processing, the inline monitoring remains accurate and robust. In some cases, a Transflection probe can already be a combined solution working well for low-fat and high-fat containing milk products. NIR Spectrometer and NIR light source remain the same for both reflection and transmission techniques.

While NIR is the workhorse of the dairy industry, advanced labs often incorporate Fluorescence, Raman, and Mid-Infrared (MIR) ATR fiber optic techniques to capture specific chemical or structural information that NIR might miss. These methods provide a higher level of "molecular specificity," making them useful for specialized monitoring in milk analysis.

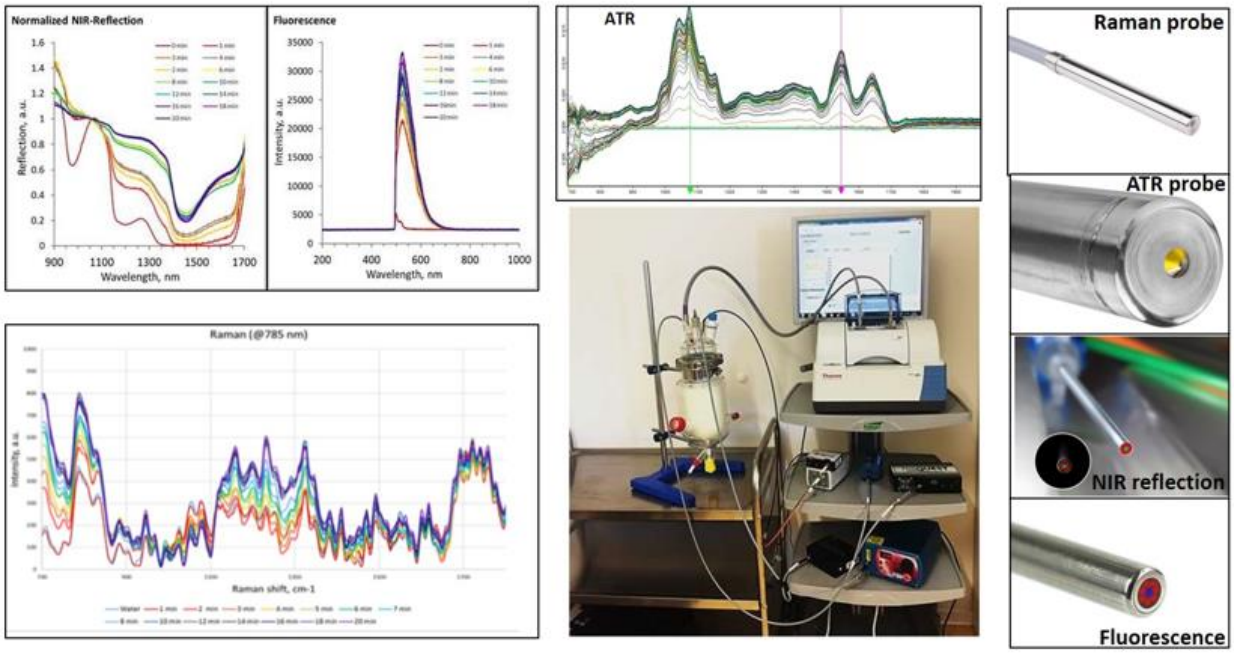

Fig. 8. Multispectral lab for milk analysis. *Image courtesy of art photonics GmbH.*

Disclaimer

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