

# A Guide to FT-NIR Spectroscopy in the Chemical Lab



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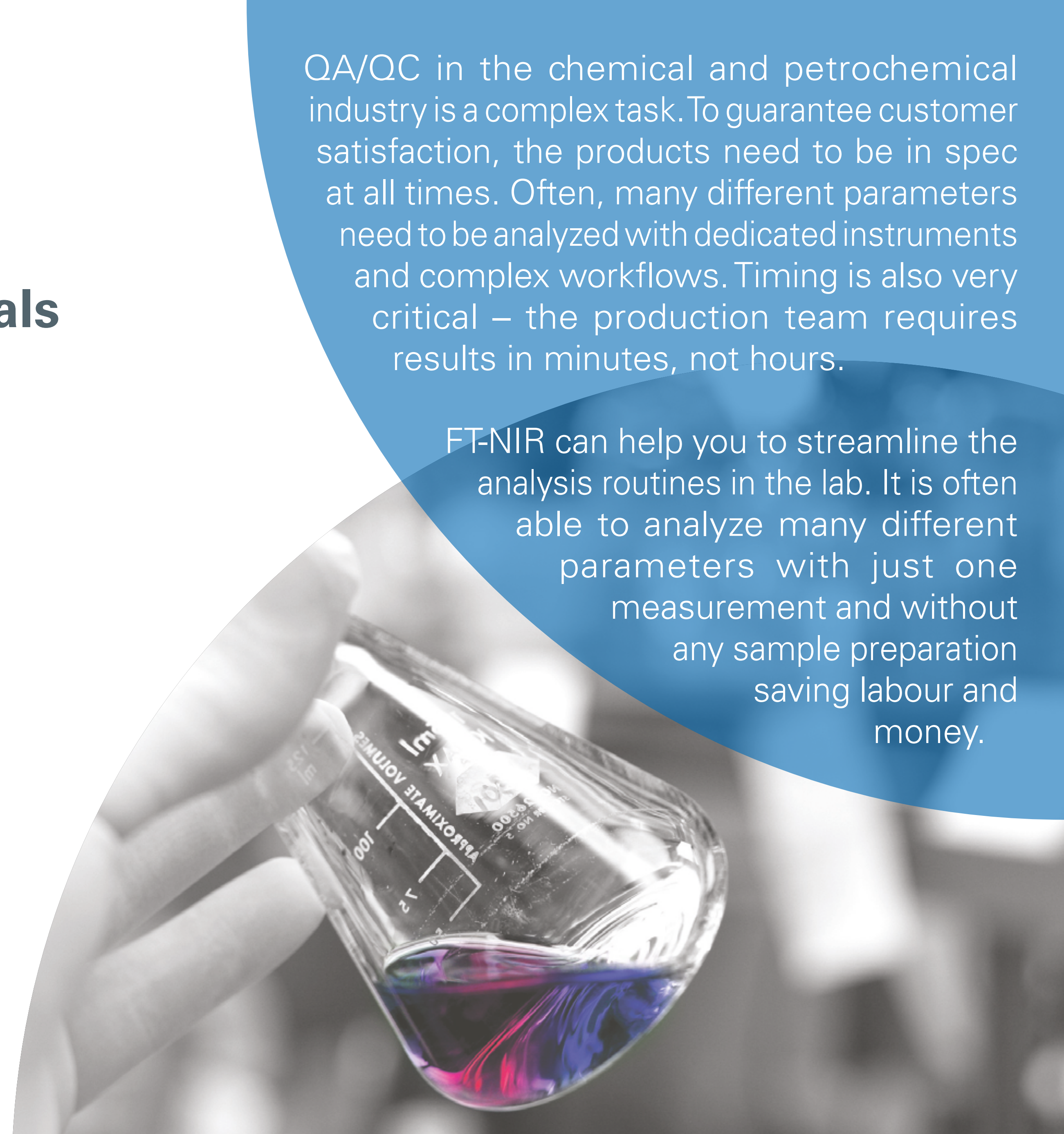
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QA/QC in the chemical and petrochemical industry is a complex task. To guarantee customer satisfaction, the products need to be in spec at all times. Often, many different parameters need to be analyzed with dedicated instruments and complex workflows. Timing is also very critical – the production team requires results in minutes, not hours.

FT-NIR can help you to streamline the analysis routines in the lab. It is often able to analyze many different parameters with just one measurement and without any sample preparation saving labour and money.





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## Why FT-NIR?

FT-NIR technology offers many advantages compared to classical wet-chemical and chromatographic analyses.

It is quick, cost-effective and safe, since no hazardous chemicals are used. It simply measures the absorption of near-infrared light of the sample at different wavelengths.

The recorded NIR spectrum is characterized by overtones and combinations of the fundamental molecular vibrations of molecules containing C-H, N-H or O-H groups, making NIR spectroscopy the first choice for the analysis of organic materials in the chemical, petrochemical and polymer industries.

[Download Application Note: Why FT-NIR?](#)

## The three biggest advantages of FT-NIR spectroscopy

...when compared to other analytical methods:

- **No Sample Preparation**

For an NIR measurement in the lab, the sample is simply filled into a glass vial or beaker, because glass is transparent in the NIR spectral region. This also allows the use of fiber optic probes.

- **Easy and Accurate Analysis**

Since NIR methods require no sample preparation, the amount of sampling error is significantly reduced, improving the accuracy and reproducibility of the analysis.

- **No Waste, No Chemicals**

In contrast to time-consuming standard analyses, the NIR method produces no wastes, causes no pollution, and requires no chemical reagents or gases, making it very cost-effective.

### What is NIR?

*Near InfraRed spectroscopy is an analysis method that uses the NIR region of the electromagnetic spectrum (800 - 2,500 nm). The NIR light interacts with the sample and results in a spectrum for evaluation.*

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## A clever investment

There are good reasons to invest in FT-NIR spectroscopy. Even when compared to analytical technologies already established in the lab, it has a huge potential for saving money in the long run.

The graph below depicts an example of the annual costs of a new FT-NIR compared to an existing HPLC. After an initial investment, which covers the cost of the FT-NIR spectrometer as well as the calibration development, you can achieve substantial cost savings from the 2<sup>nd</sup> year onwards. This calculation is just taking labor and consumables into account.

More savings can be realized in many different ways:

- **Save valuable time**

An FT-NIR analysis requires literally no additional sample preparation - no weighing, no diluting, nothing! The sample is simply filled into a cup or a vial and ready to measure.

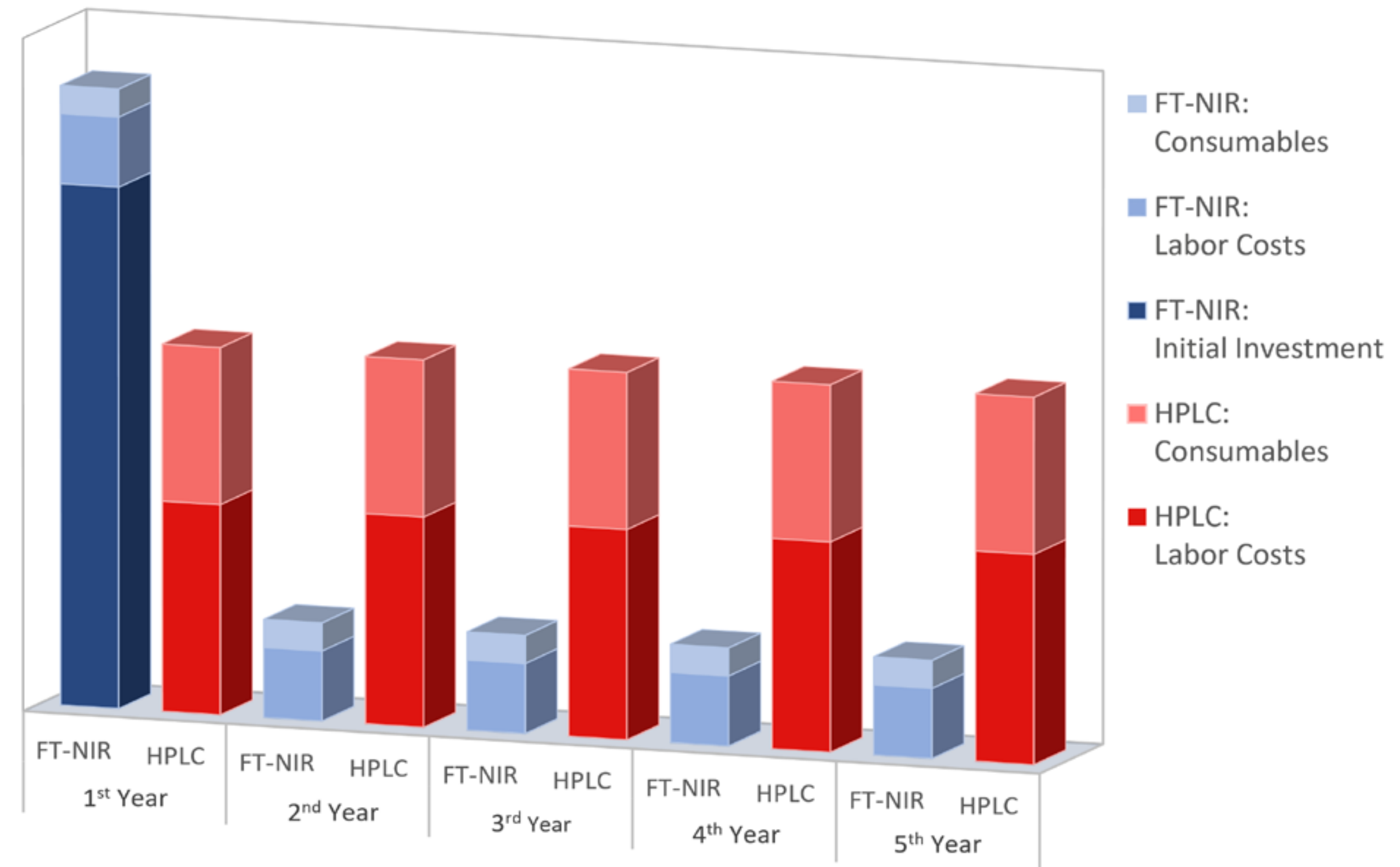
- **Improve your QC**

Due to higher the speed of a multicomponent NIR analysis compared to using several other methods, you can run far more tests at a

given time. This tight control guarantees a better-quality product and fewer costly out-of-spec batches.

- **Make better use of your „internal talent“**

By using FT-NIR spectroscopy, you can free your laboratory personnel from tedious and time-consuming analyses to be able to perform more challenging and profitable activities. This will enhance the overall output of the laboratory.





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## The Multi Purpose Analyzer

The MPA II combines several instrument types into just one, so you can always use the measurement technique that best fits your sample for optimal results:

- **Sample Compartment** with sample heater allows easy transmission measurements of liquids in cuvettes or disposable vials.
- **Integrating Sphere** with optional sample wheel for the automated analysis of solids in diffuse reflection.
- **Fiber Optic Probes** for measuring samples directly in containers, e.g. in the warehouse. Two different probes can be connected for solids and liquids.

[Download MPA II Brochure](#)

## Software controlled

The powerful, all-in-one spectroscopy software OPUS includes the most comprehensive data acquisition, processing, and evaluation functions and can be completely configured to meet your needs.

OPUS complies entirely with current GLP guidelines, featuring an extensive user management with multiple customizable access levels, global audit trail, password protected databases and a single file strategy for easy data archiving.

## MPA II

Choosing the best possible sampling method is crucial when solving a specific analysis task. With the MPA II, you have a complete FT-NIR solution at hand for your daily QA/QC work, but also for sophisticated method development studies.

Due to the modular design of the MPA II, the instrument can easily be adapted to your needs. The robustness of the instrument allows it to be placed in the laboratory and factory floor alike. Our application specialists will discuss the best configuration with you.





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## Analysis made easy

Forget tedious training courses or specialized knowledge. TANGO makes it simple for you. With its intuitive touchscreen-based user interface it, guides the operators quickly and securely through the work flow. Untrained staff can also operate the spectrometer securely and error free from day one.

Good to know: the user interface is available in more than 15 languages.

The TANGO comes in two versions, specifically targeted at the given application:

- **Transmission measurements**  
Highest precision for liquids.
- **Reflection measurements**  
Analyze solids efficiently.

[Download TANGO Brochure](#)

## Smart technology

Important for the high precision of all FT-NIR spectrometers is the exact alignment with a background spectrum.

The TANGO goes one step further: The background measurements are recorded automatically without any user intervention. This will take place even if a sample is located in the sampling position, making it 100% hassle- and error-free. So for each spectrum, the TANGO combines peace-of-mind with perfect results.

## TANGO

Sturdy housing, precise core – the TANGO connects industrial design with modern technology and intuitive touchscreen handling. The result is measurements with extraordinary precision and reliable stability.

The TANGO demonstrates how easy NIR analysis can be, not just during measurements. The housing and monitor are rugged and easy to clean – ideal for lab and at-line environments. The exchange of the light source and desiccant cartridge can be done by the user within a few seconds.





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## Chemical applications

Good chemistry is essential for creating innovative technologies.

Dealing with chemical products and materials, however, requires relevant information about their composition and properties.

A reliable, safe and economic analysis is indispensable in industrial production for the chemical industry. FT-NIR is widely used in the chemical lab because of ease of implementation and very low running costs. Also, many different parameters can be analyzed simultaneously with only one measurement.

The large number of products and manufacturing processes offer many possible applications for liquid as well as solid samples:

- Qualitative and quantitative monitoring of incoming goods

- Identification of organic solvents
- Determination of various physical and chemical parameters, such as:
  - Amine value
  - OH number
  - Acid number
  - Iodine value
  - Peroxide value

### Going online

When chemical processes become more complex, requirements for the product control, occupational safety and plant safety are huge. Here FT-NIR spectroscopy can be brought directly into the process to help you to monitor, control and automate the production.

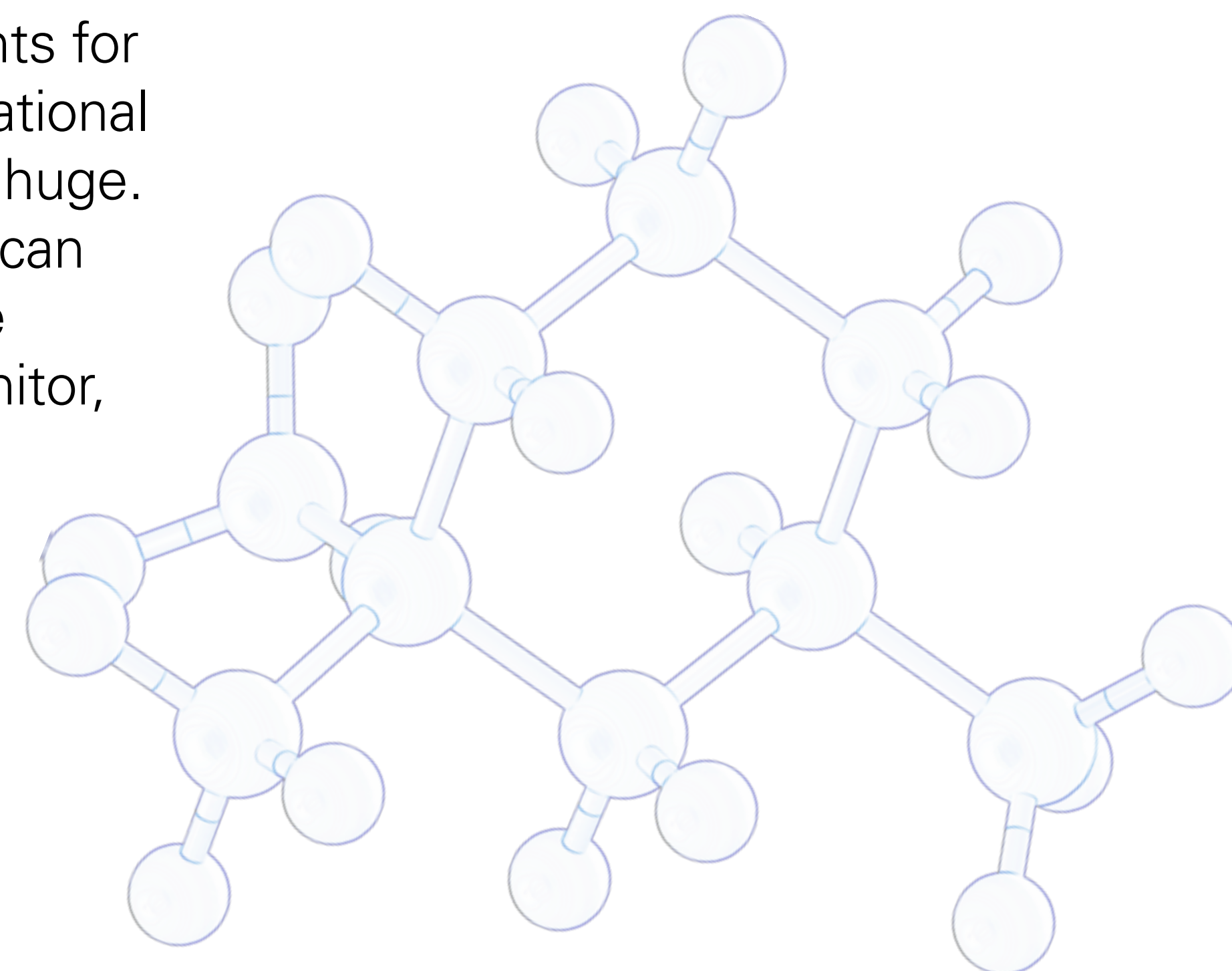
Examples include qualitative and quantitative reaction monitoring as well as endpoint determination in

following processes in the chemical industry:

- Esterification
- Hydrolysis
- Epoxidation
- Hydrogenation

Click below for more information.

[Process Applications in the Chemical Industry](#)





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## Petrochemical applications

Gasoline, Diesel and Jet fuels require extensive testing in the laboratory for production control, blend optimization and efficiency and to reduce the amount of octane giveaway.

Previously, this required many independent tests including simulated distillation (SimDis), Gas Chromatography (GC) and Knock Engine Testing. Today, with FT-NIR spectroscopy, multiple chemical & physical properties can be derived simultaneously from one sample/one spectrum in seconds.

### How does it work?

Crude oil and refinery products represent a complex mix of the most diverse hydrocarbons containing C-H, C=O, N-H, O-H and S-H functional groups. Hence, the information found in an NIR spectrum is related to the chemical composition (e.g. PIONA)

as well as to the physical properties of fuel products like octane numbers, density or vapor pressure.

These parameters can be reliably determined in the lab with FT-NIR combined with multivariate data analysis. Bruker offers an array of ready-to-use calibrations for the petrochemical industry to enable a quick and efficient start.

### Areas of Application

- Distillation of crude oil
- Steam cracker optimization
- Fuel blending

### Products and Parameters

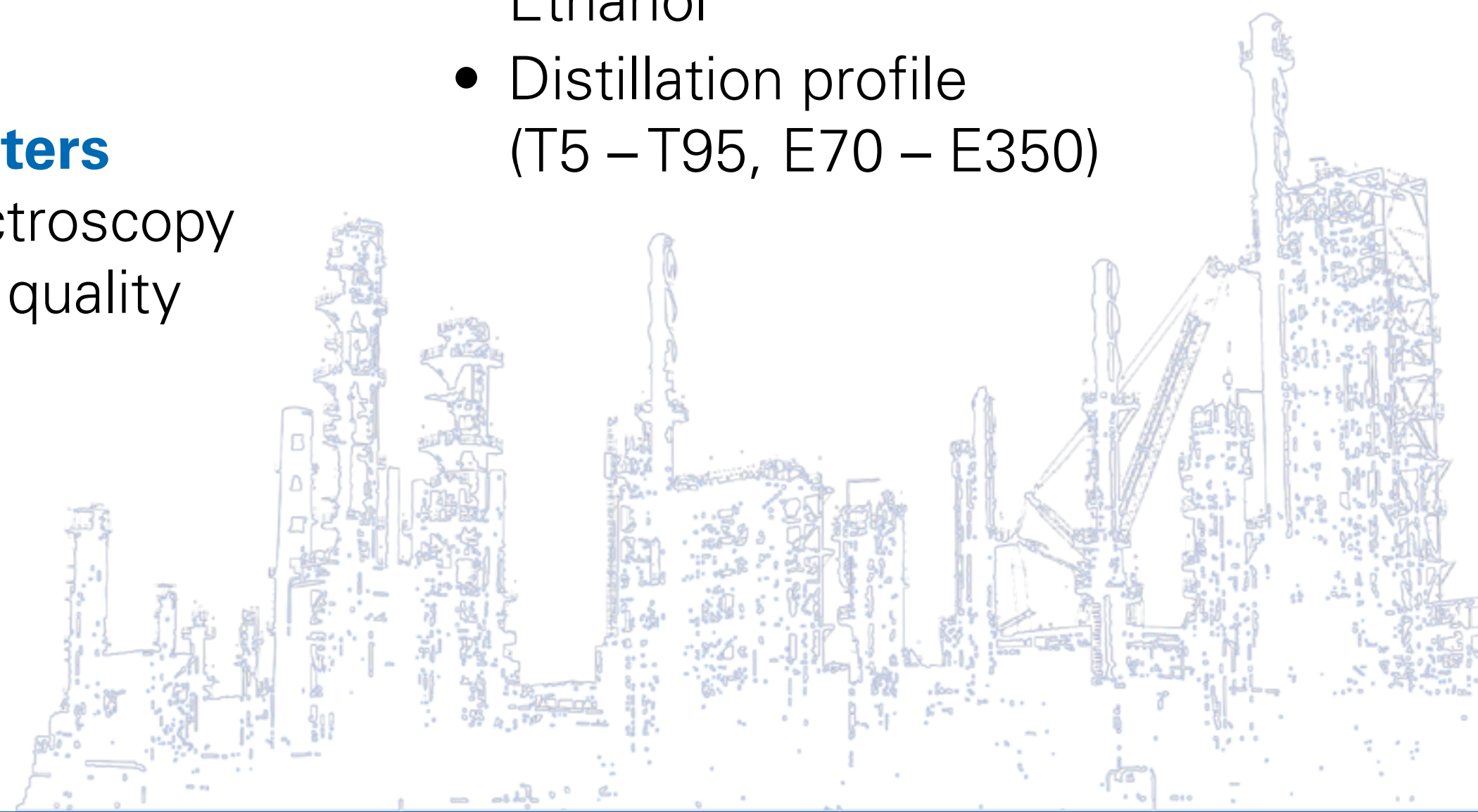
At refineries, NIR Spectroscopy is of practical value for quality control of intermediate and final petroleum products, such as:

- Reformate
- Isomerate

- Naphtha
- Gasoline
- Diesel fuel
- Jet fuel, Kerosene, etc.

Properties include:

- Octane number (MON, RON)
- Cetane number, Cetane index
- Components of PIONA
- Cloud point, Pour point
- Density
- Reid Vapor Pressure
- MTBE, Oxygenate, Methanol, Ethanol
- Distillation profile (T5 – T95, E70 – E350)





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## Polymer applications

Polymer products are an integral part of our everyday lives. High demands on the properties and quality, as well as the need for profitable production require an efficient and reliable quality control.

FT-NIR spectroscopy is today a widely used method for the analysis of polymers. By being able to look at the molecular level of a polymer, not only chemical, but also physical properties can be determined.

Typical application examples for chemical properties of polymers are:

- Acid number and OH number in polyols and polyester
- Amine value, NCO, moisture and PTMG in polyurethane
- Rubber and ethylbenzene content in polystyrenes

Physical properties of polymers include:

- Density / Molecular Weight
- Melt Flow Index / Melting Point
- Tacticity
- Viscosity

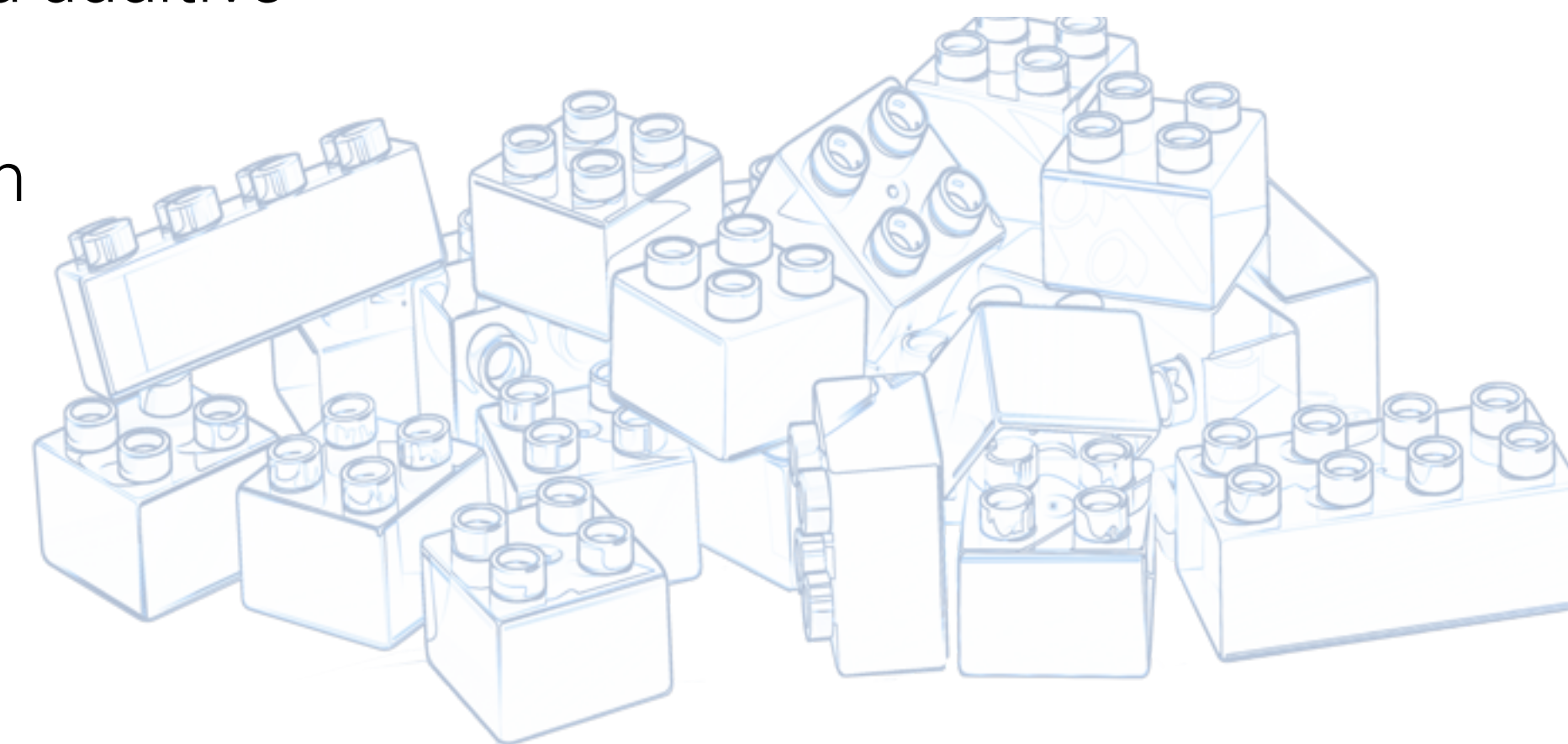
The analysis can be carried out along the production chain from monitoring the raw material up to looking at the final product before release:

- Testing raw material purity and moisture content for acceptance
- Measurement of residual solvents, monomers and additive levels
- Determining the reaction endpoint to avoid over-processing and to improve consistency.

## Accredited methodology

FT-NIR spectroscopy is today a certified method for the analysis of polymers – suitable for research, quality control, specification testing, and process control. This was acknowledged by ISO and ASTM for OH number in polyols (click below):

**ISO 15063 / ASTM D6342**  
**Standard Practice for Polyurethane Raw Materials: Determining Hydroxyl Number of Polyols by Near Infrared (NIR) Spectroscopy.**





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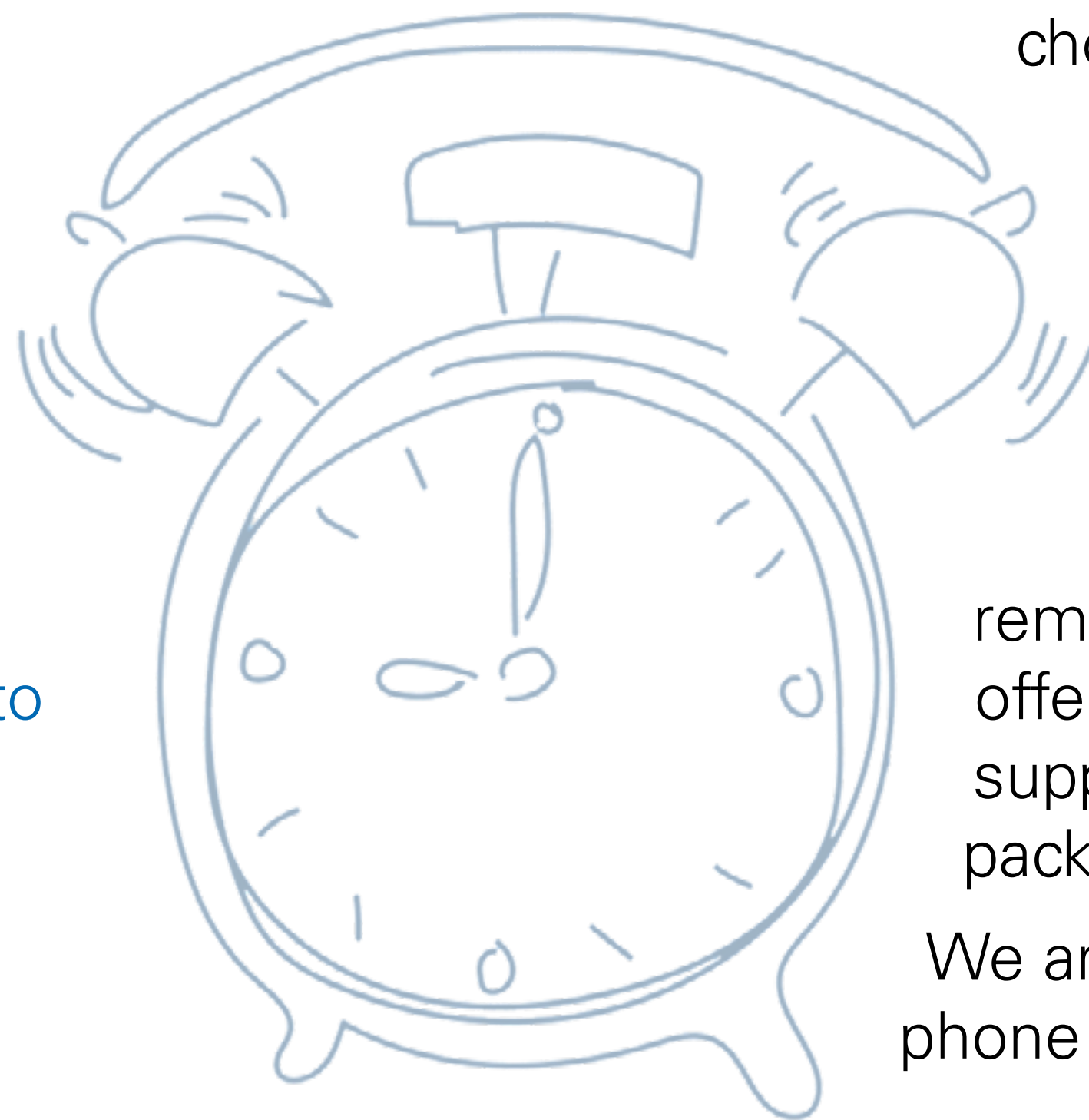
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## Summary

FT-NIR spectroscopy is the ideal tool for the laboratory or at-line analysis in any chemical, petrochemical or polymer industry.

Compared to the classical methods which often require extensive sample preparation and waste time and resources, it is fast, efficient and reliable.

It will help you optimize your analytical workflow at minimal cost and save valuable time for your lab personnel to focus on more challenging activities.



## About Bruker Optics

Bruker Optics, the world leader in FT-NIR spectroscopy, is staffed by expert scientists and engineers that have an in-depth knowledge and hands-on experience with instrumentation and applications.

Our world-wide network of experts will advise you in the selection and use of sampling accessories, choice of optical modules and software operation.

Moreover, we are there to assist you with method development either remotely or in your lab and offer customized training, support and service packages to fit your needs.

We are just an email or a phone call away!

## Web resources

If this eBook has left you hungry for more information, you will find a list of free web resources by Bruker for you to browse:

[Learn more about FT-NIR](#)

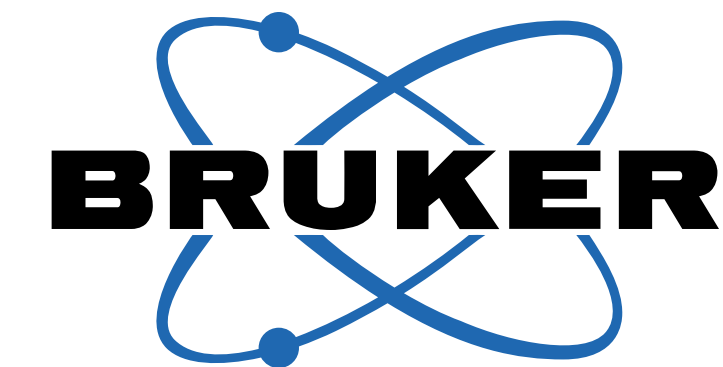
[Learn more about MPA II](#)

[Learn more about TANGO](#)

[Learn more about MATRIX-F](#)

[More than QC in the Lab? Visit our Process Website](#)





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