



BRUKER



NUCLEAR MAGNETIC RESONANCE

DISTRIBUTED LAB TOPOLOGY

Innovation with Integrity

NMR is a unique and powerful technique for chemical analysis ranging from basic identification and quantification of substances to molecular structure elucidation. With a range of NMR systems – from cost-optimized benchtop devices to high-performance floor-standing instruments – Bruker provides a powerful solution portfolio for comprehensive value chain coverage from product innovation to manufacturing. Powered by our industry-leading analysis and acquisition software TopSpin, Bruker NMR systems enable organizations to achieve a Distributed LAB Topology (DLT) in which expertise, methods, and data can be easily and quickly shared between different stages in the value chain.

NMR and Bruker

Unlike other analytical techniques – which typically concern themselves with measurements of the properties of bound electrons or entire ions – NMR spectroscopy is unique in that as it probes the magnetic behavior of atomic nuclei. This enables NMR spectroscopy to provide a unique kind of insight into the structure of molecules.

NMR spectroscopy depends on the fact that many naturally occurring atomic nuclei exhibit a magnetic moment – in other words, they behave somewhat like small magnets. When such a nucleus is held in a strong constant magnetic field and then perturbed by a weakly oscillating radiofrequency magnetic field, it responds by producing an electromagnetic signal. As in other analytical spectroscopy techniques, the response of each magnetic nucleus depends on its chemical environment. By probing a sample with an oscillating field at a range of frequencies, an NMR spectrum is obtained, revealing the sample's chemical structure.

Also, NMR is inherently quantitative and highly reproducible. Data interpretation can even be performed in a retrospective way including new analytical questions. The holistic data acquisition of NMR includes a comprehensive molecular feedback of the sample allowing for various re-processing procedures.

Since its inception, NMR spectroscopy has grown into arguably the single most widely used technique for the elucidation of molecular structure. One key advantage of NMR is that it selectively detects nuclei. Only Bruker offers a comprehensive approach: rather than focusing on either floor-standing or benchtop devices, we offer a full suite of cross-compatible NMR solutions to

provide cost efficiency, maximized solution deployment and operation capabilities at all scales of operation.

In advanced analytical applications, Bruker's high-field NMR systems set the industry standard: Our Ascend series of superconducting NMR magnets combine a number of innovative technologies for unparalleled performance, while our streamlined AvanceCore systems offer sophisticated high-field NMR analysis at exceptionally low cost of ownership.

The complete Avance floor-standing NMR product lines are highly customizable such as ^1H , ^{13}C , ^{19}F , and ^{31}P , which are commonly present in organic samples and which are typically missed by techniques such as UV-, IR- and mass-based systems.

The advantages of NMR include minimal sample preparation requirements and the ability to identify and quantify a substance against any reference standard – other analytical techniques rely on a reference standard of the same substance. Today, NMR systems are found at all levels of industry, from R&D to process optimization and quality control.



Figure 1: Fourier 80 with automation

Bruker launched the first NMR spectroscopy system in 1960 and has remained at the forefront of NMR technology ever since. Every day, countless scientists, researchers, and engineers rely on Bruker NMR systems to provide vital analytical insight at all parts of the supply chain.



Figure 2: Ascend 800 3 tower system

A Comprehensive Solution

Only Bruker offers a comprehensive approach: rather than focusing on either floor-standing or benchtop devices, we offer a full suite of cross-compatible NMR solutions to provide cost efficiency, maximized solution deployment and operation capabilities at all scales of operation. In advanced analytical applications, Bruker's high-field NMR systems set the industry standard: Our Ascend series of superconducting NMR magnets combine a number of innovative technologies for unparalleled performance, while our streamlined AvanceCore systems offer sophisticated high-field NMR analysis at exceptionally low cost of ownership. The complete Avance floor-standing NMR product lines are highly customizable tool-boxes for a variety of analytical questions in spectroscopic expert environments and in software assisted non-expert environments.

Alongside these floor-standing systems, Bruker's Fourier series of benchtop NMR systems use low-field technology to provide a compact and easy-to-use solution suited to routine and manufacturing applications. The Fourier 80, a benchtop system composed of a permanent magnet, is certainly much smaller and less heavy.

Aside from the evident price difference, the required infrastructure, logistics for the installation and maintenance diverge for the floor standing systems.

The Fourier 80 benchtop spectrometer may be placed in any temperature-stable (and if possible, vibration-free) environment. The entire set up is by magnitudes less demanding than for a high field spectrometer, in principle no specific infrastructure is required.

NMR Throughout Organizations

Industrial organizations typically deploy NMR or other analytical techniques at three major levels: corporate R&D, regional centers of excellence, and manufacturing-linked environments.

Corporate R&D

Strategic decisions for new fields of play are underpinned by analytical chemistry investigations typically performed at the corporate R&D level. This is also where standard operating procedures for the quality and process controls along the value chain are typically defined, and strategic innovation for new products occurs. This level of an organization also serves as an bi-directional interface to the academic world: new products are generally developed based on translational research from universities.

In order to develop ideas quickly from initial research to marketable products, corporate R&D teams typically use a broad analytical setup, often utilizing benchtop low-field as well as mid- and high-field NMR systems to provide versatility, speed, and sophisticated analysis where required. The translational research aspect is supported by Bruker NMR systems which are widely used in academic research.

Regional Centers of Excellence

Regional centers of excellence are expert hubs designed to facilitate new product roll-outs and volume manufacturing. Rather than focusing purely on strategic development, these facilities provide structure elucidation and in-depth screening services to support the improvement of production processes and the validation of standard operating procedures. Translating product innovation into quality and process control measures is strongly supported by staying within the same technology, but only adapting the expression of a fit to, e.g., meet spectroscopic non-expert requirements.

Regional centers of excellence typically rely on high-field floor-standing NMR systems to provide the necessary in-depth levels of analysis and the flexibility to answer a range of non-routine analytical questions.

Manufacturing-Linked Labs

Labs affiliated with manufacturing facilities are usually much more dedicated and focus on execution of routine analytical testing for incoming goods, process control, and product quality control. Typically staffed by engineers, these labs generally rely on a high degree of automation and operator independent results generation. Bruker uniquely offers benchtop NMR devices to provide identification and quantification, pre-screening, and automated basic analysis with pushbutton operation. The ability to acquire and analyze data from both benchtop and floor-standing NMR systems using the same software tool enables a Distributed Topology in which resources, data, and expertise can be efficiently shared between these different levels in an organization.

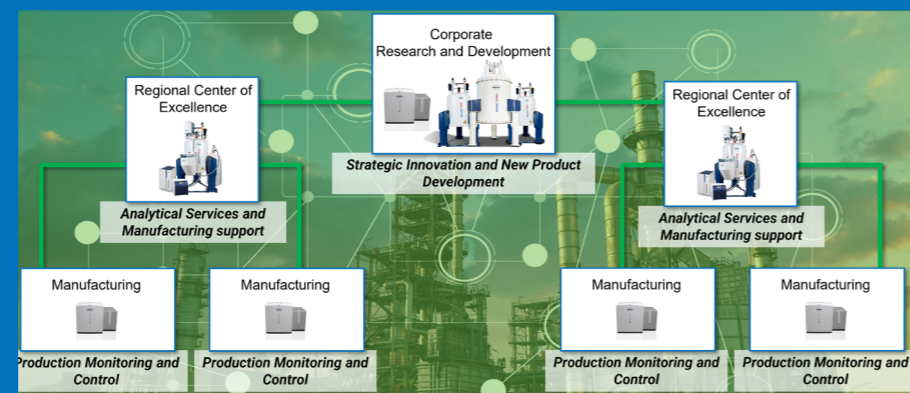


Figure 3: Distributed Topology

- METHODS that are developed in an R&D environment with the Avance series instrument can be effortlessly transferred into the manufacturing environment on benchtop Fourier units. Method validation of novel product testing is very much streamlined by staying within the same technology: NMR. Both, the transfer of R&D testing methods to manufacturing testing methods and the validation of the latter by the first one significantly reduces time-to-market of new products.
- DATA from benchtop units in manufacturing facilities can be easily accessed, analyzed, and interpreted by expert users at R&D centers utilizing a very familiar software package: TopSpin. The real-time availability of readable manufacturing affiliated testing data allows for new product roll-out monitoring and production efficiency increase measures.
- RESOURCES can be more efficiently managed, running routine-samples remotely on benchtop devices and freeing up high-investment NMR systems for more sophisticated analyses.

Bruker Distributed Lab Topology

Distributing methods, data, and resources across an organization enables significant improvements in workflow efficiency and, ultimately, product quality.

Streamlining Process Development

For organizations that use NMR, the knowledge and skill of expert users is a vital resource. Implementing a Bruker Distributed Topology enables sample queues for expert users and high-investment machines to be cut down by running repetitive samples remotely on benchtop devices. The expertise of data interpretation, also in the case of root cause investigation in failure analysis, stays centralized, but the analytical run itself isn't. Bruker Fourier series NMR systems make it easy to use procedures that were developed in R&D with single-button operation, for example, in manufacturing environments. By decentralizing work and running routine samples offsite on benchtop devices, expert users are able to focus on more sophisticated tasks. But the data can retrospectively be re-processed at any time allowing for pattern recognition if required.

Organizations that use Bruker NMR systems can dramatically accelerate their process and product development by facilitating the seamless transfer of NMR methods from R&D labs to manufacturing-linked labs. Bruker floor standing and benchtop NMR systems can be globally monitored within one software package: M-Drive. This enables management to access real-time data of sample queues, free capacities, methods assigned, and results produced.

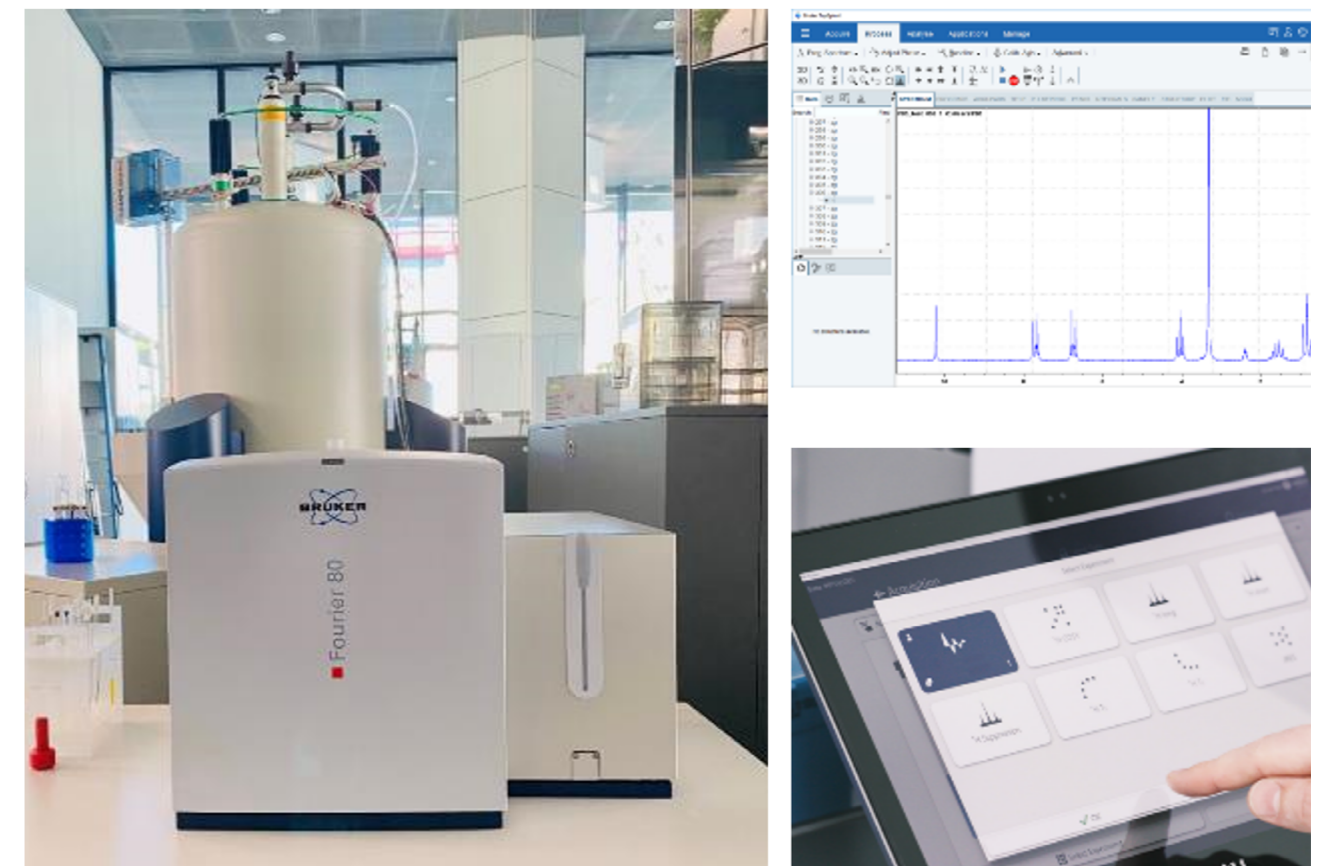


Figure 4: Fourier 80 - Low field systems with an easy to operate push button user interface

Sharing Expertise

In addition to facilitating top-down sharing of expertise, a Bruker Distributed Topology enables sample data to be efficiently sent “upstream” from manufacturing to R&D for expert analysis. In large organizations, quality control is typically carried out on a statistical basis: not every batch is necessarily screened before being used in a process. This means that when production fails, quality control personnel must look back through the process steps to pinpoint the source of the problem. Conventionally, this involves sending a sample to expert users offsite for detailed NMR analysis.

Sending samples offsite and waiting for them to be analyzed at a regional center of excellence or another R&D facility can cause major bottlenecks in production, often requiring production to be paused while a problem is identified. However, for an organization running a Bruker Distributed Topology, samples like this can be processed much more quickly. Instead of sending a sample offsite for processing, it can be processed onsite using a benchtop NMR, and the resulting data can be immediately accessed by R&D experts offsite for detailed analysis.

Bruker Fourier benchtop NMR systems allow for streamlined adoption to new product lines and analytical throughput

scaling thereof. These highly automated analytical methods can increase the testing frequency also of incoming goods leading to a stronger correlation with other production parameters. Potential issues in downstream production steps can be identified earlier if not even be predicted and mitigated before they occur. Root cause identification in failure analysis can be reduced to data analysis only as the comprehensive trace of each single sample is recorded already. Bruker TopSpin enables expert users to lend their analysis expertise wherever it is needed within an organization simply by logging in to a familiar interface and accessing the relevant data. Using a Distributed Topology with Bruker NMR systems seamlessly automates the process from sample to report, providing rapid answers to analytical questions. Distributing expertise in this way can significantly shorten time to result in routine production processes, and the event of problems.

Consistency and Comparability

One of the key advantages of NMR is data consistency. By contrast, for example, gas chromatography results are notoriously difficult to compare due to the aging of the column and detector, requiring comparison of the histories of different instruments. This is not the case with NMR: results from

different systems can be compared easily and to a very high level of detail. This is uniquely utilized in a geographic sense by comparing analytical results from different sites, but also in a historic sense by comparing different batches of production. Harmonizing methods and using NMR throughout an organization bring an inherent compatibility advantage, eliminating the time used for translating results from one technique to another and so decreasing time to market for new products.

Using Bruker NMR systems for analysis at an organization-wide level brings other advantages. Daily instrument check-ins are automated: simply load a daily check sample, and it is run daily and stored again. This further enables simple auditing because the condition of a given NMR instrument can always be proven.

With Bruker NMR systems, training is simplified. By relying on a single piece of software for all analyses, money spent training personnel on software and products can be dramatically reduced. In addition, using Bruker NMR consolidates service and maintenance requirements to a single point of contact, further reducing complexity and saving money.

NMR Software

All Bruker NMR systems – from floor-standing to benchtop – are unified by our industry-leading acquisition and analysis software, TopSpin. Using the same piece of software to operate NMR systems at all scales opens the door to significant improvements in organization-wide efficiency through what we call a Distributed Lab Topology (DLT). Any experiment set up in TopSpin can be imported into the push button graphic interface GoScan.

GoScan

Designed for the Fourier 80 and AvanceCore, [GoScan](#) serves as an intuitive and easy to handle software. Standard and customized experiment setups and NMR acquisition are made accessible also to less experienced NMR users, students for instance. Ranging from the push button usage of pre-defined experiment setups to the option to individually create sophisticated experiments, GoScan is meant to serve users of any level of expertise. In combination with a sample-changer, measurements can be run in automation and their status observed immediately.

TopSpin

[TopSpin®](#) is Bruker's standard NMR software used in a wide range of workflows. Starting with the control of the spectrometer up to the processing and analysis of multidimensional NMR spectra. The acquisition interface provides easy access to vast NMR experiment libraries including standard Bruker pulse sequences and user generated experiment libraries, for both routine and advanced NMR users. TopSpin provides numerous options for setting up and optimizing NMR experiments, making the setup of sophisticated experiments simple and efficient. For users who must be compliant with the GxP regulations, the software supports the various principles of data integrity.

Mdrive qNMR GxP

Potency determination, absolute compound purity assessment, identity testing, residual solvent, moisture analysis, relative response factor calculation... Have you thought about using quantitative NMR as a one-stop solution? [Mdrive qNMR](#), new tool for potency/purity determination, streamline this process with a fully automatic workflow from experiment submission to report, making it the ideal solution for both experts and non-experts working in an industrial environment, where an efficient quality control process is key to gain time to market.

Check the Most Comprehensive Portfolio of [NMR Software](#)

Figure 5
Top Spin for processing

