Nuclear Magnetic Resonance

- Solutions for Life Science and Analytical Research

Innovation with Integrity

NMR

Fourier

Dedicated high-resolution NMR spectrometer delivers affordable NMR for all your common applications in education and routine chemistry research

Fourier brings NMR within everyone's reach. It delivers powerful performance at extremely compact size, low weight and most importantly, minimal cost. With its new Fourier probe technology and a unique push-button, power on/off concept, ease of siting and handling is guaranteed. Designed and built by the world's NMR market leader, Fourier unique qualities include the industry standard operating software, TopSpin™. TopSpin's various tools for exploring the world of NMR make Fourier the ideal solution for chemistry education and routine analysis. Researchers have access to numerous pre-defined 1D and 2D experiments and interactive, automated processing tools help to transfer spectroscopic data into a corresponding report.

Easy sample loading on the SampleXpress Lite

Benefits

- Affordable NMR spectrometer for chemistry education and small molecule analysis
- Industry standard TopSpin software
- High throughput SampleXpress Lite 16 position sample changer
- Proven IconNMR software for automation control
- New robust Fourier NMR probe for easy handling
- 1D/2D proton and carbon NMR for every chemist

Sample setup with the intuitive IconNMR interface

AVANCE III HD

The AVANCE™ III HD is the ultimate NMR platform for life-sciences and materials research. Robust, automated and easy-to-use, it is the ideal NMR analysis system for the pharmaceutical, biotech, and chemical industries, for metabonomics, materials science, molecular diagnostics, and much more.

The AVANCE III HD is the newest generation in the very successful AVANCE series, which has established Bruker as the clear technological and market leader in NMR and pre-clinical MRI worldwide. The AVANCE III HD spectrometer architecture is designed around an advanced digital concept which provides an optimized pathway for high-speed RF generation and data acquisition with highly modular and scalable transmitters and multiple receiver channels.

The AVANCE III HD spectrometer benefits from a new RF synthesizer with significantly increased digital integration, incorporating a lower phase noise local oscillator (LO) and a high speed DA converter running at 960 MHz. This enables extended digital RF power settings up to NMR frequencies of 1.2 GHz. Together with the new high dynamic range and high sensitivity preamplifiers, the AVANCE III HD demonstrates improved artefacts, fully exploits the increased sensitivity of the latest NMR probe technology and delivers sensitivity improvements of up to 30% for the most demanding of applications.

Benefits

- NMR Thermometer™
- Minimum event time: 25 ns
- High-speed RF generation and data acquisition
- Scalable transmitters and multiple receiver channels
- High-dynamic range and digital resolution
- Large-bandwidth digital filtering

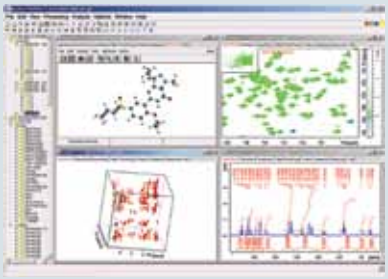
Ultra-High Field AVANCE III 850 MHz NMR system

AVANCE III HD NanoBay

The most fully integrated state-of-the-art NMR spectrometer ever

The AVANCE™ III HD NanoBay is the most comprehensively integrated, state-of-the-art NMR spectrometer ever produced. The NanoBay's bold, innovative design manages to reconstruct Bruker's high-performance AVANCE III HD NMR spectrometer technology within an exceptionally compact enclosure.

It delivers high-productivity with highest quality NMR information for pharmaceutical and industrial chemists, as well as food analysis, diagnostics research and other small molecule applications.



AMIX™ provides a collection of powerful tools that enable statistical and spectroscopic analyses of your NMR data, and delivers increased productivity for a wide variety of applications, such as metabolomics, small molecules research and mixture analysis.

IconNMR™ is the graphical user interface for fully automated acquisition and processing. This productivity tool excels whenever large numbers of samples accrue, or where multiple users access your spectrometer.

Benefits

- Ultra compact, innovative high-end NMR spectrometer
- Available at 300 and 400 MHz
- Full HD NMR electronics
- Broadband / Full automation
- Built-in 'CryoProbe ready' preamplifiers
- Easy siting in small analytical laboratories
- TopSpin™ - intuitive routine user interface
- NMR Thermometer™ ready
- High-fidelity NMR information for a wide range of chemical applications

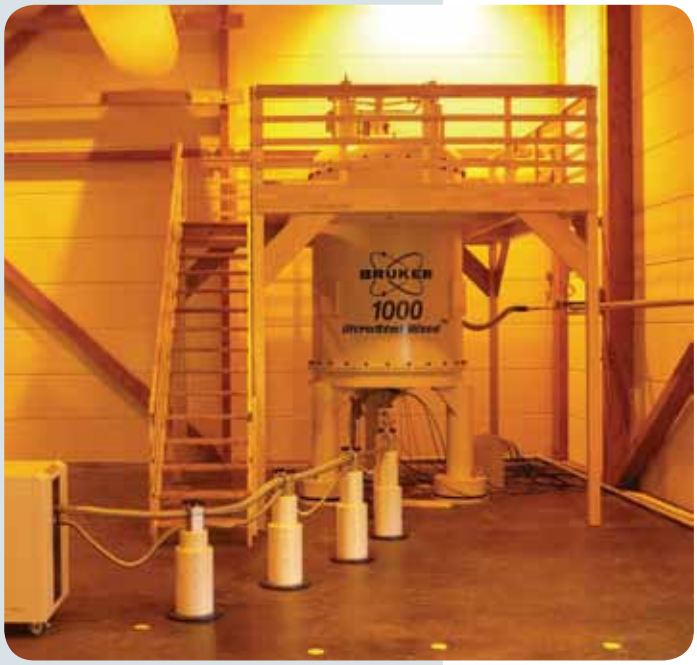
AVANCE III HD NanoBay 400 MHz spectrometer

AVANCE 1000

Bruker is proud to provide the world's highest field NMR system of highest sensitivity and dispersion to the scientific research community. The AVANCE 1000 pushes biochemistry, structural biology and molecular research to new frontiers.

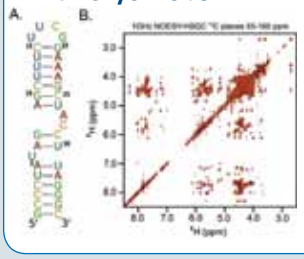
The first AVANCE 1000 NMR system equipped with a CryoProbe has been installed at the new 'Centre de RMN à Très Haut Champs' in Lyon, France.

- 1 GHz NMR system with 23.5 T persistent superconducting magnet
- Standard bore, 54 mm diameter
- UltraStabilized™ sub-cooling technology, achieving the highest field and most compact magnet coil at this field strength
- Proprietary jointing technology enabling high current and high-field joints with minimum resistance for maximum field stability
- 5-mm triple-resonance CryoProbe, enabling unique 1 GHz NMR applications
- 1.3-mm, 2.5-mm & 3.2-mm double and triple resonance MAS probes, enabling unique 1 GHz NMR solids applications



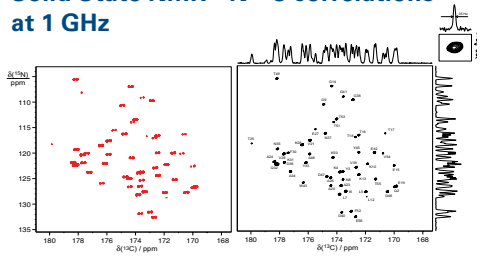
World's first 1GHz (23.5 T) UltraStabilized magnet installed at Centre de RMN à Très Haut Champs, Lyon, Fr. Courtesy: Prof. L. Emsley.

RNA, 3D NOESY-(^{13}C)-HSQC at 1 GHz with CryoProbe



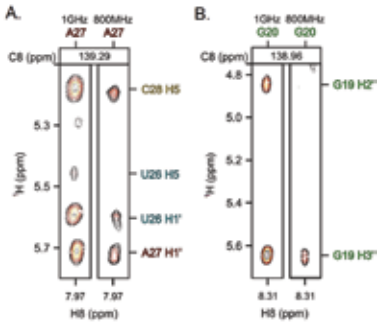
NMR structure determination of the conserved secondary structural motif of 23S rRNAs by John King, Christos Shammas and Vasudevan Ramesh, (University of Manchester).

Solid State NMR ^{15}N-^{13}C correlations at 1 GHz



NCO correlation recorded on U[^{15}N,^{13}C]-microcrystalline GB1 without (left) and with (right) a S3E J-decoupling block; 60 kHz MAS, T1max=40 ms, T2max=50 ms, NS=48, exp. time=17 hrs.

RNA, 1 GHz vs 800 MHz



Comparison of ^{13}C planes of the 1 GHz and 800 MHz 3D NOESY-(^{13}C)-HSQC spectra. (**A**) (139.29ppm) (A27) (**B**) (138.96 ppm) arising from G20 H8 proton and the NOEs observed thereof to G19.

Acknowledgements:

Dr. Moreno Lelli, Dr. Józef Lewandowski, Dr. Guido Pintacuda, Dr. Anne Lesage, Dr. Benedicte Elena, and Prof. Lyndon Emsley with CRMN, Lyon, France.

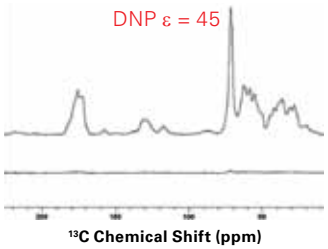
DNP-NMR Spectrometer

Sensitivity boost for biomolecular NMR

263 GHz DNP - NMR Spectrometer

Dynamic Nuclear Polarization (DNP) experiments transfer polarization from electron to nuclear spins, enhancing sensitivity and dramatically reducing signal averaging time. Bruker AVANCE DNP-NMR spectrometers are designed specifically for solid-state NMR, delivering unsurpassed sensitivity for exciting new applications.

DNP CPMAS of ^{13}C-Proline



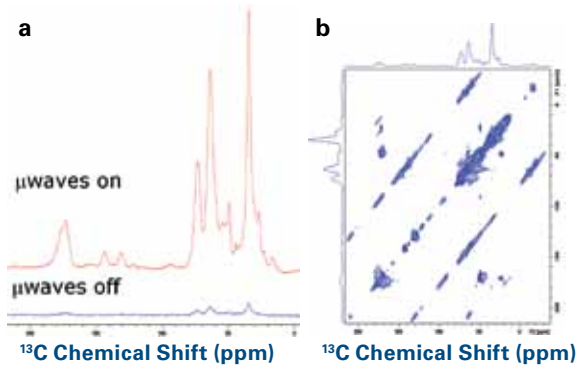
Courtesy of Prof. Ann McDermott, Columbia University

^{13}C CPMAS spectra with and without microwaves irradiation of a micro-crystalline yeast Triose Phosphate Isomerase (TIM) frozen solution with 20 mM TOTAPOL. 32 scans, 2 s recycle delay, 9 kHz MAS, 100 K sample temperature, 400 MHz ^{1}H frequency.

Benefits

- DNP-enhanced solid-state NMR experiments at high field
- Polarization enhancement yields up to a factor of 80 gain in sensitivity, to date
- Unique high power 263 GHz micro-wave source with easy-to-use software-controlled high-power gyrotron (9.7 T)
- Microwave transmission line designed for optimum beam propagation to the sample
- Low-temperature MAS probe technology with cold spinning gas supply and built-in wave guide
- 395 GHz (600 MHz ^{1}H) and 528 GHz (800 MHz ^{1}H) spectrometers in development

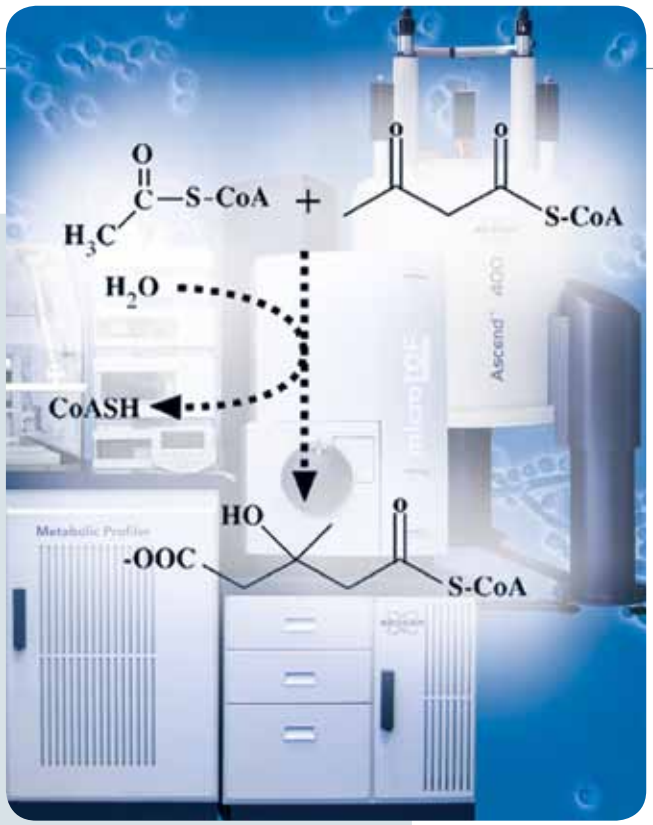
DNP on membrane proteins



Courtesy of Prof. David Weliky, Michigan State University

DNP experiments on membrane-associated HIV gp41protein with uniform ^{13}C,^{15}N labeling at Ala-6 and Gly-10. (**a**) ^{13}C CPMAS spectra with and without µwaves showing a factor of 22 DNP signal enhancement at 100 K, 8 kHz MAS, 32 scans, 5 s recycle delay. (**b**) DNP-enhanced DARR ^{13}C-^{13}C correlation experiment with 15 ms mixing time, 32 scans, 8 kHz MAS, and 200 points in f1.

Metabolic Profiler



Metabolic profiling and fingerprinting is a key process in the pharmaceutical industry for studying drug efficacy or toxicology. In clinical research, metabolic profiling helps to identify biomarker compounds for early disease detection and monitoring, and enables researchers to study the effects of drugs in biological systems in a rapid and robust method.

Integrated Analysis

The Metabolic Profiler™ is a dedicated, integrated LC-NMR/MS solution for metabolic analysis featuring an AVANCE NMR spectrometer and a micrOTOF-Q II™. This system provides a simple, easy-to-use and inexpensive base for acquiring the spectroscopic data needed for basic metabolic profiling. The system delivers the integration of automated sample handling, acquisition, collection and archiving of your data, and enables the comparative and statistical analysis needed for your research.

Data Management

SampleTrack™ is an Oracle®-based information system that utilizes SQL tools for organizing, searching and archiving sample information, which can simplify experimental control of large sample sets.

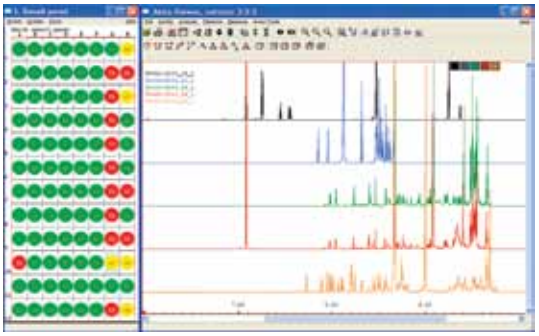
Statistical Analysis

The AMIX program provides a comprehensive range of powerful tools that enable statistical and spectroscopic analyses of both your NMR and MS data. AMIX features Pattern Match - which can define spectral patterns in multiple ways and project these to spectra. In addition, the Multi-Integration features can be used to identify and quantify metabolites in complex mixtures.

Reference Compound Spectral Database

The most complete metabolite NMR spectral database available which contains over 17,000 spectra of the most common endogenous metabolites. By taking into account the effects of pH, field strength and by using one as well as two dimensional NMR data, the database enables the assignment of metabolites in biofluids, cell extracts and tissues in a unique and unambiguous way. Linking the database to AMIX enables automatic investigations, such as matching to mixture spectra. Direct integration into statistical data evaluation is also possible.

Analysis with AMIX



AMIX™ analyzes data and is linked to the Spectral Database for further comparative analysis.

Magnets

Bruker has specialized in the design and production of magnets and cryogenic systems for a wide range of applications, becoming the world's largest manufacturer of superconducting magnets for NMR. Bruker is engaged in every aspect of the magnet business including research and development, production and testing, individual site planning, as well as service and support.

UltraStabilized

UltraStabilized™ is our innovative magnet technology for Ultra-High Field NMR up to 1000 MHz. This proprietary technology provides reliable, stable operation at reduced helium bath temperature and ambient pressure.

US²

The US² represents the efficient combination of Bruker's renowned magnet technologies (UltraStabilized™ and UltraShield™) for enhanced system performance and siting flexibility at Ultra-High Field strength.

Ascend

This new magnet line at 400 to 850 MHz incorporates the key technologies of the well-established UltraShield™ Plus magnets, with new innovations for superior performance. The Ascend™ magnet design features advanced superconductor technology, enabling the design of smaller magnet coils, resulting in a significant reduction in the size of the cryostat. Ascend magnets are therefore easier to site, safer to run and have lower operational costs. These high-performance systems are ideal for structural biology research and materials research applications.

Ascend 500, 600, and 700 MHz systems

Room Temperature Probes

X Observe Probes

These probes are optimized for observation of X-nuclei. They are available in selective or broadbanded versions for double, triple and quadruple resonance experiments, including automated tuning and matching.

^{1}H Inverse Probes

The inner coil of these versatile probes, in multinuclear or selective configuration, is fully optimized for ^{1}H observation at highest sensitivity with optimal lineshape. The available configurations and choices of X-nuclei are identical to those for X Observe Probes.

Inverse MicroProbes

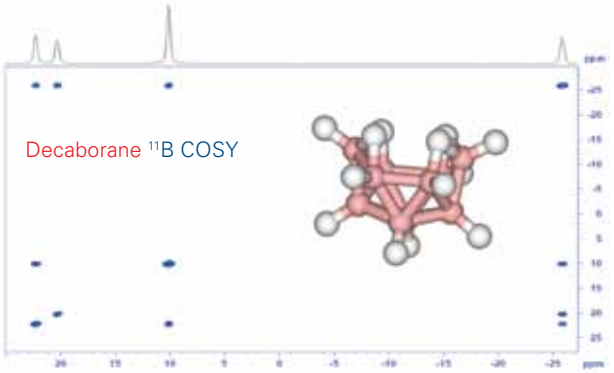
For highest ^{1}H sensitivity per mole of substance, e.g. in natural products applications, Bruker offers 1- and 1.7-mm ^{1}H/^{13}C/^{15}N fixed-frequency probes.

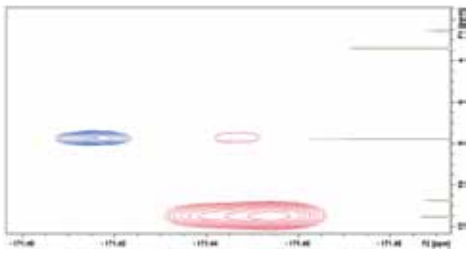
SmartProbe

SmartProbe

The SmartProbe™ delivers highest sensitivity on both the multinuclear and proton channel. The SmartProbe design exclusively features a broadband frequency channel enabling fully automated applications on protons and the widest range of X-nuclei. This unique probe technology enables fluorine applications including ^{19}F observe with ^{1}H decoupling and vice versa.

SmartProbe Applications with X-nuclei





Comparison of the ^{19}F, ^{1}H HOESY and HMBC experiment. While the HOESY spectrum has a correlation to the proton of the heterocycle, the HMBC shows a correlation to the NH protons.

CryoProbes & Prodigy

CryoProbe Prodigy

CryoProbe™ technology has delivered the single largest increase in detection sensitivity ever achieved in the evolution of NMR equipment. The factor 3-4 jump in sensitivity enables the use of correspondingly smaller sample quantities that are impractical with conventional probes, or enables the user to increase sample throughput up to 16-fold.

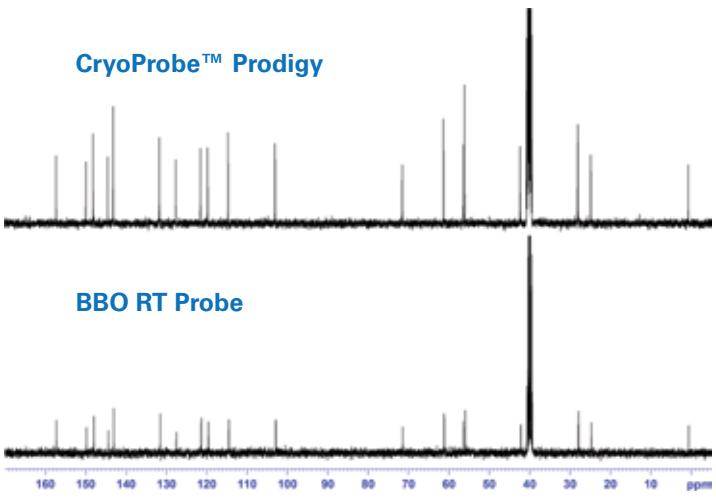
Product Lines

Bruker offers the largest range of CryoProbe configurations from 400 MHz to 1000 MHz, including proton optimized probes such as our 1.7- and 5-mm inverse triple-resonance probes, as well as 10-mm dual ^{13}C observe probes.

The 1.7-mm Micro-CryoProbe offers an increase in sensitivity per mole of more than an order of magnitude compared to a conventional 5-mm probe. For optimal X-nucleus detection we offer the 5-mm Quad CryoProbe in $^{13}C/^{31}P/^{19}F/^{1}H$ and $^{15}N/^{13}C/^{31}P/^{1}H$ versions. All high-resolution CryoProbes are equipped with a ^{2}H lock and a Z-gradient. A ^{1}H micro-imaging CryoProbe is also offered to enhance the study of sample structure and properties in the micrometer range.

CryoProbe Prodigy with pump and control unit

SNR Comparison with Conventional RT Probe



Comparison of the ^{13}C-sensitivity of a standard BBO probe with the CryoProbe Prodigy at 400 MHz. Sample: 50 mM quinine, 32 scans each.

Prodigy

CryoProbe Prodigy is a new, revolutionary CryoProbe that delivers tremendous boosts in sensitivity at an affordable price. Costing significantly less than a conventional CryoProbe, the broadband CryoProbe Prodigy uses nitrogen-cooled RF coils and preamplifiers to deliver a sensitivity enhancement over room temperature (RT) probes of a factor of 2 to 3 for X-nuclei from ^{15}N to ^{31}P. The sensitivity gain on the proton channel exceeds standard probe performance by a factor of 2 or more.

The CryoProbe Prodigy is now also available as triple resonance inverse probe (TCI).

Solids Probes

Our comprehensive range of the most advanced solids probes is ideal for inorganic and biological samples using experiments such as CP, d.CP, MQMAS, or REDOR.

Maximal spinning rates are 70 kHz for the ultra-high speed 1.3-mm MAS probe for materials science, 30 kHz for the 3.2-mm triple-resonance E^{free} MAS probe for protein research, and 15 kHz for the 4-mm HR-MAS probe with Z gradient for metabolomics studies.

Our BioSolids probes are based on one of two technologies, TL_2 or E^{free}. For optimum performance these probes are configured as fixed frequency triple resonance probes, most often requested for proton, carbon and nitrogen. TL_2 probes yield the best overall sensitivity with high ^{1}H sensitivity for inverse detection experiments.

E^{free}

E^{free} probes are specifically designed to minimize RF heating. The two coil configuration provides enhanced sensitivity for ^{13}C and ^{15}N and the highest tuning and matching stability for safe, long term experiments. Minimized RF heating ensures the integrity of your protein, even while operating at room temperature.

1.3-mm MAS

The 1.3-mm probe product line provides the highest spinning speeds coupled with high-sensitivity and RF fields. Where sample heating might become an issue, convenient low power decoupling can be employed.

Efree probe

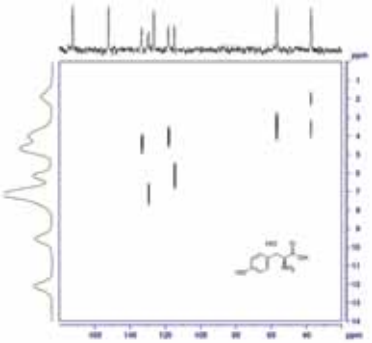
TL_2

TL_2 technology is the choice when high-decoupling fields are needed for optimum decoupling in J-coupling based experiments and when sample heating is not an issue. TL_2 probes are best used for dry and non-salty samples, or samples that are kept in a frozen state.

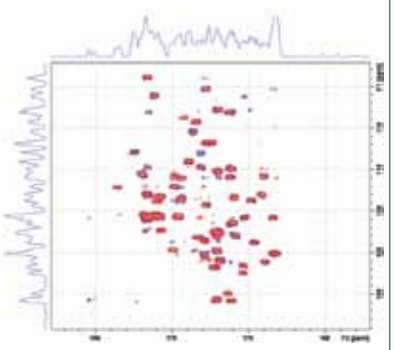
1.9-mm MAS

The new 1.9-mm MAS probe now enables fast spinning of nuclei less sensitive than ^{19}F and ^{1}H, offering 42 kHz spinning frequency at 10 µL active sample volume.

NMR using fast magic angle spinning



700 MHz 2D FSLG-HETCOR of L-tyrosine-HCl. Spinning frequency was 42 kHz, RF field for FSLG was 140 kHz. Projections are 1D ^{13}C CP/ MAS and ^{1}H wPMLG-5 spectra, respectively. Note that only directly bonded ^{1}H – ^{13}C correlations are visible.



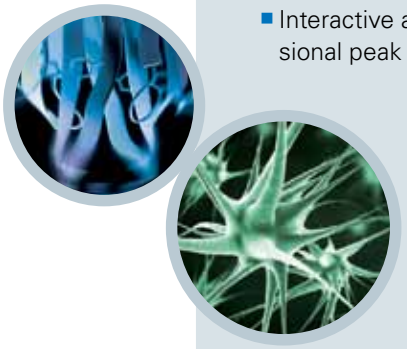
NCO PAIN CP with ultrafast sample rotation. Spectra with 3 ms (red) and 6ms (blue) mixing time for long distance contacts in GB1 at 60 kHz rotation, 5°C with 75–80 kHz, ^{13}C, ^{15}N and 15 kHz on ^{1}H. (Lewandowski et al. JACS 129, 728 (2007))

TopSpin

Ideal for first-time spectrometer users as well as routine users, TopSpin's different acquisition tools make it easy for both beginner and expert to find their way to an NMR spectrum.

TopSpin provides a wealth of data processing visualization and administration features, including:

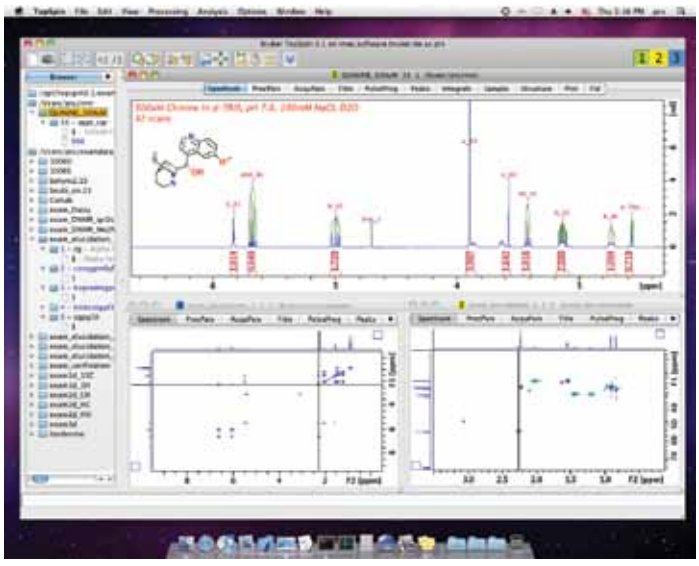
- Comprehensive functionalities for dealing with 1D to 5D data including automatic forward/backward or delayed linear prediction
- Inverse Fourier transform processing of rows, columns, planes and subcubes of nD datasets
- Interactive and automatic multi-dimensional peak picking and integration.



Features

- PC-standard user interface offers easy accessibility for Windows® and Linux® users
- Comprehensive functionalities for processing, displaying and analyzing single and multi-dimensional spectra
- Intuitive acquisition
- Non-uniform sampling
- Small molecule characterization
- BioTools™ - Biomolecular NMR made easy
- Method development environment
- Result publishing, predefined and user-defined layouts
- Lineshape analysis for solid-state NMR, including dynamic NMR
- Regulatory compliance support tools (audit trailing, electronic signature, autoarchiving)
- Special licenses for students and universities

TopSpin User Interface



TopSpin 3.1 on Mac

TopSpin for Mac OS X

Entirely programmed in the native Apple Mac OS X environment, the new TopSpin software caters to MAC users' familiarity with the unique and intuitive characteristics of that operating system, while maintaining the proven capabilities, look and feel of TopSpin. Incorporating a comprehensive range of NMR data analysis, processing and simulation features, TopSpin includes modules for efficient small molecule characterization and structural biology research.

Automation

AVANCE™ NMR systems meet the most demanding automation needs by streamlining every aspect of NMR analysis, including sample submission, sample preparation, automatic probe tuning, data acquisition, processing, data distribution and archiving. Depending on the laboratory's needs or goals, automation may involve high-throughput screening, overnight automation or multi-user open access.

IconNMR

This productivity tool excels whenever large numbers of samples are submitted for standardized experiments, or when many users access the spectrometer. IconNMR™ supports sample changers and sample preparation robots. The user can set up or supervise measurements remotely via a Web browser from a desktop or pocket PC.

SampleJet

SampleJet™ changer for 300-700 MHz NMR systems offers both high-throughput as well as individual sample capabilities in a single NMR sample changer. Its versatile design can accept samples from five 96-position racks, allowing batch analysis of up to 480 tubes. In addition, the SampleJet easily accepts single tube samples via a separate carousel that can hold up to forty-seven 1-, 1.7-, 3- and 5-mm tubes.

SampleCase

SampleCase™ is the first NMR automation solution that provides easy, safe and convenient access to fully-fledged NMR automation at user height. Ensuring simple random access automation without the need for steps or ladders, it also enables manual insertion and ejection of samples with the simple push of a button. The user-friendly system can be fitted to almost any Bruker NMR magnet.

SampleXpress

SampleXpress

Bruker's easy-to-use, cost-effective solution for medium-throughput automation in NMR routine and research applications. Its compact, exceptionally integrated design drastically reduces sample exchange times to just a few seconds, making SampleXpress™ ideal for optimizing throughput in standard NMR service laboratories running 30-100 samples per day. In addition, efficiency is maximised thanks to interchangeable, easy-fill cassette modules that can be loaded off-system and in parallel with current experiments. The system is also equipped with integrated bar code reader for automatic sample identification.

SampleCase

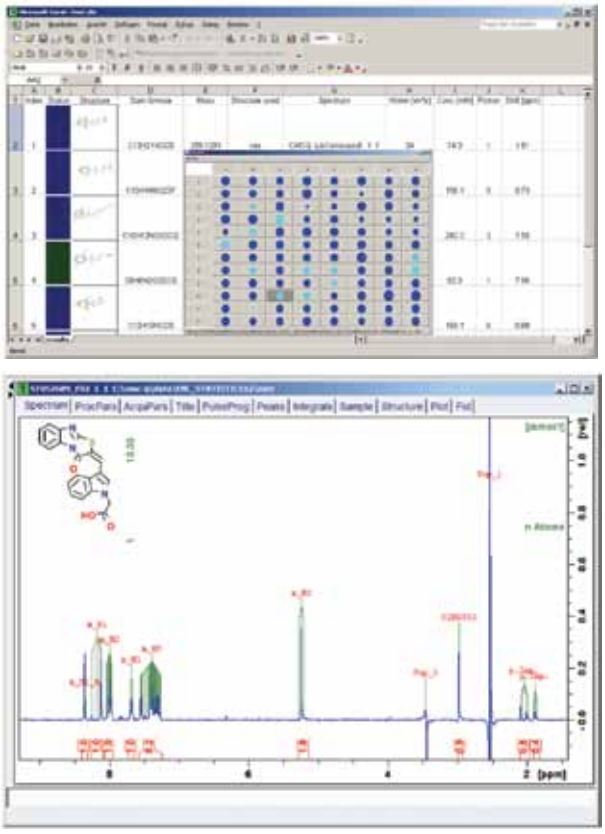
Complete Molecular Confidence (CMC™)

CMC-i: Structure Consistency Analysis

Only complete computational NMR spectral analysis provides a safe assessment of the consistency between a given structure and its ^{1}H NMR spectrum. Finally those tedious manual procedures have been overcome. Fully automated optimization of predicted spectral parameters to match experimental data using iterative spectral analysis is now a reality.

- Complete NMR spectral analysis yielding fully assigned spectra and highly accurate spectral parameters extracted from data, even for overlapping signals and strongly coupled spin systems
- Benefits from PERCH's highly sophisticated algorithms for predicting chemical shifts and couplings and optimizing them to match the experimental data using iterative quantum mechanical spectral analysis
- Extremely safe assessment of the consistency between a given structure and its ^{1}H NMR spectrum data based upon the quality of the fit and the similarity between predicted and actual spectral parameters, with optional use of HSQC information
- Highly reliable estimation of sample purity

CMC-q



Single and multiple result view

CMC-q: Absolute Quantification

Complete Molecular Confidence for quantification (CMC-q) is a complete workflow solution that facilitates automatic NMR-based quality assurance in batches.

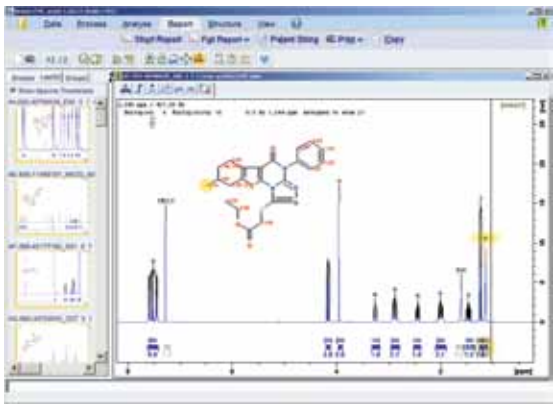
- CMC-q provides quick access to automated NMR quality assurance and quantification of larger batches of samples. Delivering accurate, precise information on sample concentration and water content in typical screening samples, CMC-q also marks questionable structures and provides a suggestion for spectral assignment. This is ideally complemented with LC-MS information such as that derived from Bruker's SmartFormula program.
- Operating on a file-in, file-out basis, the user supplies an input file describing the samples to be measured, and receives an output file of results.
- The spectra interpretation function can also analyze individual datasets and prepare spectra for publication or for further analysis.

CMC-assist: Data Interpretation and Workflow Streamlining

The most powerful software tool for interactive, assisted NMR data analysis is now available. Designed for NMR end-users, CMC-assist efficiently extracts information from complex NMR data, conducts assessments and generates detailed reports for direct transfer to publications, patents and lab journals. CMC-assist not only excels as an off-line analysis interface but its automated NMR interpretation power can also be used to generate results directly at any Bruker NMR instrument equipped with the latest control software, making it the most efficient and streamlined NMR workflow on the market.

- Seamless integration with Bruker spectrometers
- State-of-the-art analysis engine, powered by modern human logic emulation algorithms
- Automatic results may be refined manually
- Automatic data analysis includes:
  - Integration and ^{1}H number determination
  - Multiplet analysis
  - Structural assignment
  - Consistency statement
  - Concentration
- Reports include detailed PDF and multiplet string in different journal formats
- Windows, Linux or Mac operation systems are fully supported

CMC-assist & CMC-se



CMC-assist User Interface

CMC-se: Structure Elucidation

CMC-se is an NMR software package for simple and efficient structure elucidation of small molecules. With its innovative approach, CMC-se accelerates the spectroscopist's workflow during the elucidation process by automating many of the key analysis and interpretation steps. In combination with Bruker's Avance™ NMR spectrometer product line, CMC-se is the only elucidation tool that integrates high-quality NMR data acquisition with sophisticated software analysis. CMC-se is available for the major operating systems: Windows®, Linux® and Mac OS® X.

- Simple and efficient structure elucidation of small molecules in drug discovery and natural products research
- Automates many of the necessary analysis and interpretation steps
- Seamless integration of NMR acquisition and sophisticated software analysis
- Enables both accomplished researchers and beginners to expedite the elucidation of unknown substances in diverse pharmaceutical and chemical applications
- Organizes the data for a molecule into a single project, and provides unique graphical tools for data visualization and interpretation

Assure

Assure RMS-Raw Material Screening

Impurities and adulterants in starting materials pose potential health threats when present in the manufacturing of pharmaceutical APIs and drug products. These same impurities and adulterants may also result in lower production yields and increased product purification. Screening starting materials by NMR using Assure - Raw Material Screening identifies problem samples prior to use and prevents costly manufacturing mistakes. Designed for GMP and GLP environments, Assure - Raw Material Screening provides a traceable record of sample analysis and results. Applications include pharmaceutical and chemical production and analytical reference standards.

Quantification

Category	Concentration	Status	Match
Active Ingredient	99.64%	✓	✓
Adulterant	0.36%	✗	✓
Impurity	0.00%	O	
Unknowns	-		

Fail % relative to total integral

Compound	Concentration	Status
Hydrocodone	99.64%	quantified
Phenetole	0.36%	quantified
Solvent	0.00%	Not quantified

Quantification results of main components and impurities are reported in a simple to read format with a user defined 'pass/fail' threshold.

Features

- System suitability test for GMP/GLP labs
- Automated data acquisition
- Automated quantitative and qualitative analysis
- Automated report generation
- QC report - a 'pass' or 'fail' report
- Detailed expert report - total analysis
- Lock-out mode for access-limited users
- Convenience features
- Sample SBASE/KBASE
- Customizable

Assure SST - System Suitability

Assure-System Suitability Test (SST) is the ideal tool for any NMR spectroscopy laboratory. In full automation, the NMR spectrometer is validated regularly for instrument performance and optimized before you run your samples.

Choose from a list of available individual tests to perform lineshape and sensitivity measurements on your liquid-state NMR spectrometer that will run at a time convenient for your facility.

Probe-specific parameter settings enable use on practically any liquid-state NMR probe.

Assure-SST's Temperature Calibration feature calibrates AND adjusts the temperature of the sample to the actual desired value. Accuracy in temperature provides optimal results for spectral reproducibility from instrument to instrument.

- Fully automated performance validation
- Instrument optimization
- Monitors performance of 'walk-up' instruments
- Enables NMR specialist to produce more results
- Improves data quality
- Meets GLP requirements

JuiceScreener

The JuiceScreener™, combined with its SGF Profiling™ technique, delivers huge amounts of information from one single experiment, instead of multiple individual analysis steps. This provides higher throughput and reliability than conventional techniques, leading to a significant reduction in cost per sample. This enables up to 5 times more sample investigations with no change in budget, resulting in an improved and more comprehensive quality control screening program.

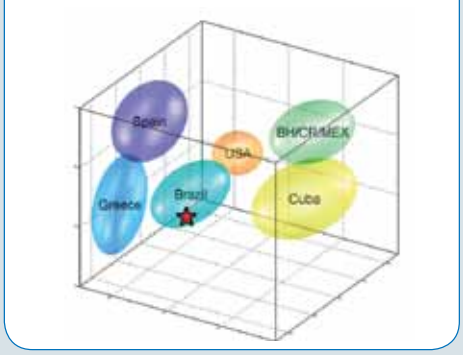
Push-Button Routine

SGF Profiling is a fully automated push-button routine that needs no interaction from the operator. From sample bar code registration, preparation and handling, to data acquisition and statistical evaluation, all steps are under the control of SampleTrack™, Bruker's laboratory information system.

Spectroscopic Database

Screening is based on a constantly updated, extensive spectroscopic database that includes thousands of NMR spectra from mainly authentic juices. Currently the database includes about 40 different fruit types from more than 50 production sites worldwide. In addition, the database also provides access to hundreds of small molecule compounds for further analysis of unknown ingredients.

Origin Authentification of Orange Juice



Features

- Fully automated push-button NMR solution including evaluation and reporting
- Simultaneous absolute quantification of all relevant organic ingredients for juice assessment
- High-throughput with minimal sample preparation
- Reduced cost per sample
- Reliable screening method providing targeted and non-targeted multi-marker analyses
- Enables the detection of unexpected fraud
- Screening is based on an extensive NMR spectroscopic database of more than 8000 reference juices, obtained from production sites all over the world
- Complex statistical models enable the analysis of: origin authenticity, species purity, fruit content, false labeling, production process control and sample similarity

Hyphenation

Major tools for small molecule research and mixture analysis include HPLC, SPE, NMR and MS. Bruker offers hyphenated systems to meet various research needs. While NMR can be used to investigate the complete mixture, LC-NMR can analyze the individual compounds separated by the chromatography. An LC-NMR interface can easily be added to any NMR system from Bruker thereby also enabling hyphenated LC-(SPE)-NMR(/MS) applications. By combining the structural resolving power of NMR for the separated compounds with the mass accuracy of the micrOTOF, we can offer the most complete system for structural analysis available today.

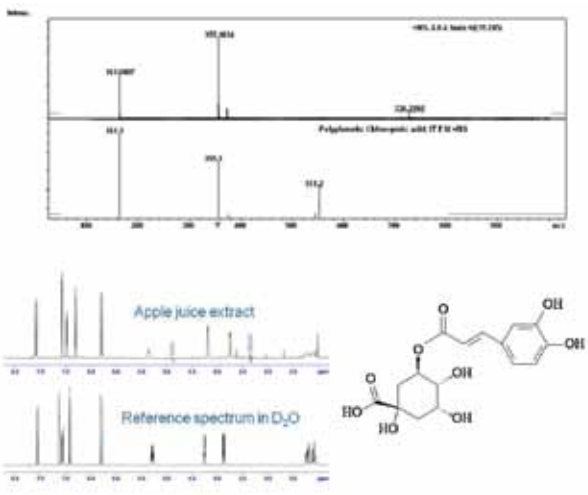
Hyphenated system including sample preparation, NMR, LC and MS

LC-(SPE)-NMR

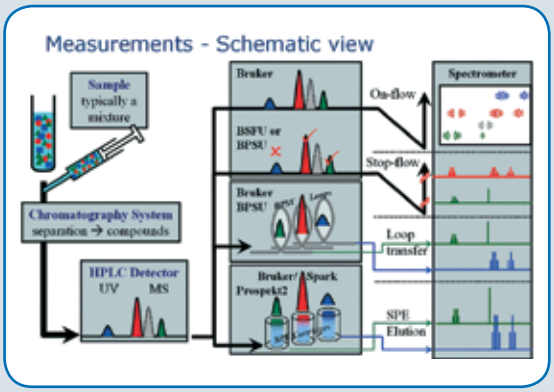
Two different methods for coupling are possible: either by coupling the chromatography system directly to the NMR spectrometer, or by the intermediate collection of the samples. Direct coupling can be performed as stopflow or on-flow analysis. For intermediate collection loop-storage or collection on solid phase extraction (SPE)-cartridges is possible.

The use of SPE provides an efficient interface between chromatography and NMR even enabling the analysis of low level metabolites.

LC-SPE-NMR-MS Results



LC-(SPE)-NMR-MS of Apple Juice high resolution mass spectra from m/z 355.1034 (upper part) of chlorogenic acid and the comparison with ion trap library (lower part) ^{1}H NMR spectrum of chlorogenic acid and the comparison with reference compound commercially available.



Immediate Access to Latest Technologies

Contract Bruker Analytical Services

Everyone can now benefit from Bruker's latest technologies, instrumentation, and unmatched experience in analytical applications. We offer supporting services that include advanced high-resolution NMR and mass spectrometry applications. Our customers can benefit from access to the latest developments in the field through Bruker's cooperations with academic and industrial research labs. Our experts can also assist you with special customized projects.

Benefits

- Short and long term support increases project handling capacity
- Latest, most advanced Bruker technologies
- Unique analytical expertise and knowledge
- Method development and feasibility studies

Advanced NMR Services

- Structure verification and elucidation
- Reaction and purity control
- Quantitative analysis
- Variable temperature experiments
- Screening methods for pharmaceutical and clinical research
- Food quality control
- Juice analysis using SGF-profiling
- Metabonomics studies
- Natural product analysis

Additional Analytical Services

- Mass Spectrometry & Imaging
- EPR (ESR) Spectroscopy
- TD (Time Domain) NMR Spectroscopy
- X-ray Diffraction, Crystallography & Fluorescence
- FT-IR Spectroscopy & Microscopy
- Raman Spectroscopy & Microscopy
- LC-(SPE)-NMR/MS

Customized Projects

When additional measures are needed, our technical experts will discuss the range of special capabilities available to you. Whether it is a short term project where specialized equipment is a necessity, method development is required or feasibility studies are needed, we can help you with our extensive resources.

High-Performance Power Supplies

High-Voltage Power Supplies

Bruker high-voltage power supplies find their main applications in IOT- and Klystron-based RF transmitters in Particle Physics. Our power supplies provide high-voltages of up to 50 kV at broad range, from 1 kW up to several Megawatts. The compact solid-state design is based either on the latest switch mode technique or, in the case of highest power applications, based on SCR (Thyristor) control.

Klystron power supply for the MAMI C race track microtron, Mainz University, Germany.

High-Current Power Supplies

Bruker high-current power supplies are employed in industry and particle physics research worldwide. Our high-current power supplies, available for pulsed or DC, monopolar, bipolar or four-quadrant operation, deliver high-currents of up to 30.000 A. Based on the latest switch mode technology they ensure optimum efficiency and enable stand-alone, fail-safe operation. The option of linear mode regulation provides maximum stability and minimum noise and fluctuations from 1% to better than 1 ppm (part per million).

For high-power applications our high-current power supplies benefit from SCR (Thyristor) control. We offer single- and multi-channel supplies starting in the 100 Watt range going up to several Megawatts.

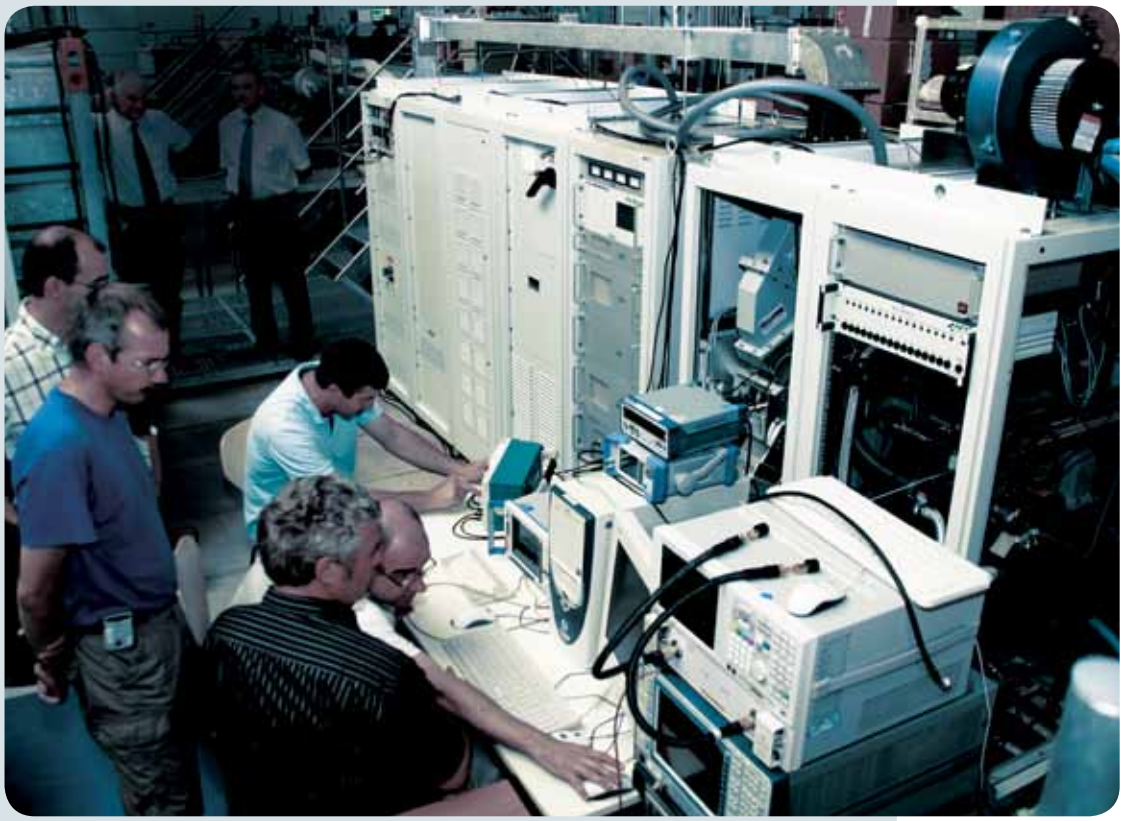
RF Transmitters

Bruker Radio Frequency Transmitters are established in nuclear physics applications all over the world. Our high-voltage power supplies, capable of emitting power from 100 Watt up to 300 kW and more, benefit from modern switch mode design for optimum efficiency and feature SCR (Thyristor) control to handle the highest power applications.

Choose from single or stacked solid-state amplifiers, whilst IOT amplifiers deliver optimum peak power conversion efficiency.

For arc protection our emitter tubes operate with defined stored energy, with optional solid-state crowbar circuits to protect the sensitive elements.

Start-up and operating procedures are handled automatically ensuring stand-alone, fail-safe operation, while a solid-state safety system ensures maximum protection for the transmitter elements and the user applications.



RF IOT high-power transmitter at ELBE FZD Rossendorf, Dresden, Germany.