



Agilent NMR Chemistry Solutions

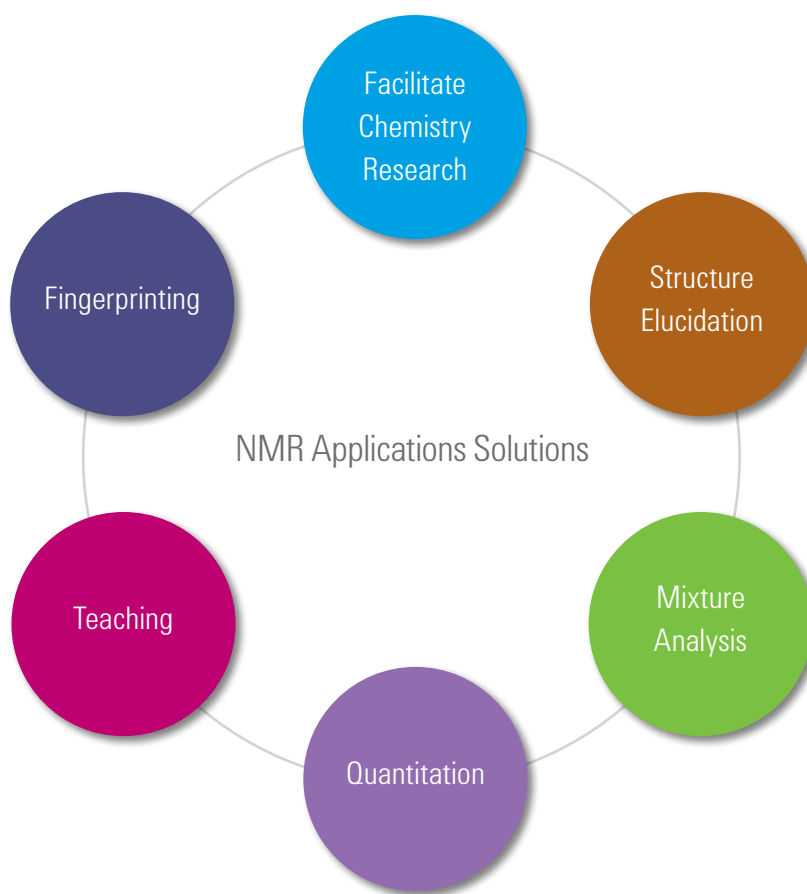
## STRUCTURE FOR YOUR NMR WORKFLOW

The Measure of Confidence



**Agilent Technologies**

# ANSWERS FOR EVERY APPLICATION



The uses of NMR for chemistry research and education are extensive and quite diverse. You might use your system to support hundreds of medicinal chemists, to teach an undergraduate chemistry course, or to support a QA/QC laboratory. Maybe you routinely need to determine the concentration of unknown samples

with high precision, or test the purity of food samples. You may even take on structure determination for a series of unknown compounds, or a combination of these tasks depending on the day of the week.

This diversity of NMR analyses required to optimally support small molecule chemistry presents many

distinctive challenges. However, one thing is for sure. You expect your NMR vendor to provide a complete set of tools that support optimized and easy-to-use workflows for fast, accurate and reproducible results. Agilent's NMR systems uniquely deliver these solutions for all of your NMR spectroscopy needs.

# A COMPLETE NMR SOLUTION

## Superior performance combined with ease-of-use

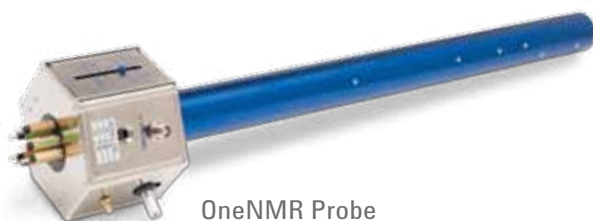
With the powerful combination of high productivity VnmrJ 3 software, the innovative DD2 console series, the revolutionary OneNMR probe, and versatile automation options, Agilent has assembled a complete solution for the applications you run every day.



400-MR DD2 System



7510-AS Autosampler



OneNMR Probe



VnmrJ 3 Software

## EASY-TO-USE WORKFLOWS FOR CHEMISTRY RESEARCH

For high-throughput and day-to-day chemistry workflows Agilent offers a complete, optimized and easy-to-use system that ensures reliable operation and maximizes productivity.

- VnmrJ 3 software presents a targeted and intuitive user interface that is easily adapted to different user skill levels.
- Our well designed, intelligent automation solutions provide for robust, continuous operation with minimal downtime.

### Facilitate Chemistry Research

The Agilent DD2 system serves organic chemists who rely on NMR for information about chemical structure, sample purity, reaction progress, or physical characteristics with a versatile, flexible, and intuitive system.

- The OneNMR probe delivers uncompromising performance simultaneously for  $^1\text{H}$  &  $^{13}\text{C}$ .
- Exceptional console linearity enables you to determine absolute concentration of any sample easily and reliably without using a standard.
- Adaptive NMR eliminates guesswork and maximizes spectrometer efficiency by reliably predicting the time needed for  $^{13}\text{C}$  and 2D experiments.

### Fingerprinting

NMR in a QA/QC environment, generating certificates of analysis for example, demands a highly robust and reliable system that delivers reproducible data.

- VnmrJ's versatile batch submission tools minimize effort and simplify operation.
- Automated reporting and sample documentation provide easy access to a complete history of sample data.
- The linear and highly stable DD2 system enables fast, accurate and precise quantitation without internal or external standards.

### Teaching

Whether you are introducing students to NMR instrumentation and data collection techniques or supporting advanced researchers, Agilent's collection of flexible software tools makes user training simple and straightforward.

- System protection tools prevent damage from user errors and avoid unscheduled downtime.
- Easy access to advanced experiments and modern pulse sequences maximizes productivity for both advanced students and teachers.
- Create or remove multiple user accounts with a spreadsheet to easily manage large numbers of students.

## OPTIMIZED WORKFLOWS FOR ADVANCED RESEARCH

For more advanced applications, The DD2 System supports high data quality, improved ease-of-use and reliable operation for complex workflows.

- The OneNMR probe enables you to collect all of the data required for structure analysis of organic molecules without changing probes.
- Agilent's DD2 architecture and parallel RF design represent integral elements of every Agilent NMR spectrometer, providing uncompromised performance.
- The DirectDigital receiver digitizes at 80 MHz, delivering outstanding dynamic range, sensitivity and rock solid baselines across myriad applications.

### Mixture Analysis

Precise results are crucial for complex mixture analysis, such as food science work or polymer studies. The Agilent DD2 System with VnmrJ 3 delivers accurate and precise diffusion data.

- Our best-in-class DOSY software package with modern pulse sequences delivers more complete analysis of minor constituents, resulting in more accurate identification of mixture components.
- Pulse sequences offering convection compensation and powerful solvent suppression schemes determine highly accurate diffusion coefficients even for challenging samples.
- Multi-exponential fit of diffusion attenuation & peak-by-peak or point-by-point fitting lets you extract useful information even in the case of spectral overlap.

### Structure Elucidation

NMR in a QA/QC environment, generating certificates of analysis for example, demands a highly robust and reliable system that delivers reproducible data.

- A complete and modern pulse sequence library, including Hadamard transformation-based fast experiments, puts the tools you need at your fingertips.
- Interactive experiment setup & parameter inheritance saves time and effort by eliminating the repetitive entry of identical sample information.
- Adaptive NMR validates experimental choices by reliably predicting time required to complete complex experiments.

### Quantitation

Whether you are introducing students to NMR instrumentation and data collection techniques or supporting advanced researchers, Agilent's collection of flexible software tools makes user training simple and straightforward.

- Point and click software tools for quantitative NMR (qNMR) enables high quality absolute concentration determination by any user.
- Flexible batch submission tools improve throughput for busy laboratories.
- Convenient and customizable reporting tools deliver absolute concentration values in user-defined formats, such as a spreadsheet to make data analysis fast and easy.

# OPTIMIZE EVERY OPPORTUNITY

Robust sample automation; compact magnets; highly stable, linear, and sensitive consoles and probes; and powerful software all combine to deliver unparalleled ease and performance for small molecule chemistry research.

## Systems

Compact and efficient magnets minimize space requirements and cryogen costs. DD2 console technology provides the most stable and linear NMR platform.



The Agilent 400-MR is the instrument of choice for laboratories that require a compact and easy-to-use instrument for fast and reliable analyses day in and day out.



## Probes

High performance probes from the revolutionary OneNMR probe to very sensitive small volume cold probes and the  $^{13}\text{C}$  optimized XSens probe deliver outstanding results.



Agilent's MicroSample Cold Probe is the best solution for the characterization of quantity-limited samples.





# GREATER THAN THE SUM OF THE PARTS

## Automation

Flexible sample automation solutions extend the workday by ensuring robust unattended operation.

The Agilent 7510-AS NMR autosampler improves productivity and simplifies sample handling in your NMR laboratory. Each removable carriage holds up to twelve samples and supports random access. Load one carriage while running another.

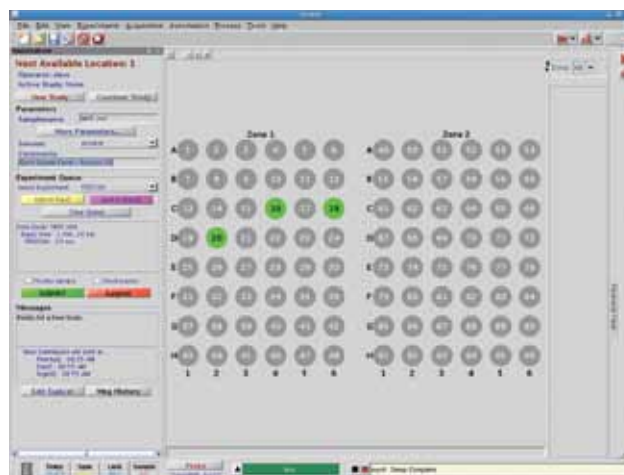
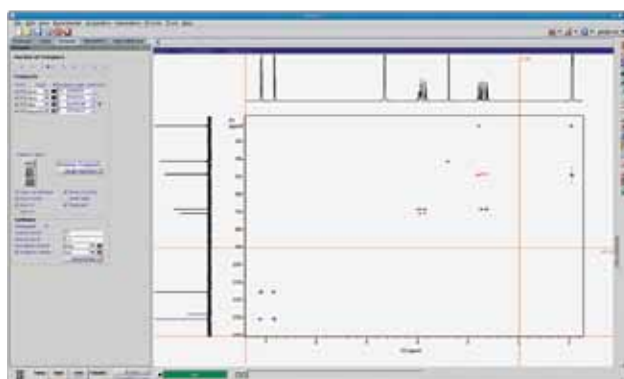


The 7600-AS is compatible with all standard NMR sample tubes from 1.7-10 mm in diameter and lengths up to 9 in. No special caps or spinners are required allowing you to freely use automation for all your liquids NMR samples. The SCARA robot with its sealed joints will provide years of reliable and essentially maintenance-free operation.



## Software

VnmrJ 3 software thinks like a chemist and lets you work the way you want. The sample-centric design ensures that data gathered from multiple experiments is always associated with the sample. This new way of thinking enables you to get to an answer more quickly.



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