Agilent 400-MR DD2 System

NMR TECHNOLOGY DESIGNED FOR YOU

The Measure of Confidence

Agilent Technologies

COMPLETE SAMPLE-TO-ANSWER SOLUTIONS

The Agilent 400-MR DD2 system is the platform of choice for laboratories requiring a compact and easy-to-use instrument that delivers fast and reliable results day in and day out.

The 400-MR DD2 provides unmatched productivity for diverse chemical applications by combining easy-to-use software with the outstanding performance of this second generation DirectDrive and DirectDigital spectrometer architecture. Push-button experiments, along with straightforward processing and data export capabilities, make the 400-MR the best choice for compound detection, quantification and structure confirmation.

Advanced automation accessories including autosamplers and the proprietary OneNMR probe enable users to take full advantage of the 400-MR's capabilities. These technologies are seamlessly integrated with sample-centric data management in VnmrJ software.

400-MR Magnet

NMR Console

7620-AS Autosampler

VnmrJ Software

OneNMR Probe

AGILENT'S PRODUCTIVITY ADVANTAGE

Versatility in a Single Probe

The OneNMR Probe uses a novel hybrid approach to deliver the performance advantages of both the classic carbon (direct detection) probe and the highly sensitive proton (indirect detection) probe. It provides all of the data required for structural analysis of organic molecules.

Flexible Sample Automation

NMR autosamplers extend the workday by allowing unattended operation and eliminating idle time between sample changes. The 7620-AS (96 samples) and 7510-AS (12 samples) random-access autosamplers are compatible with the widest possible range of tubes. On-board sensors monitor key aspects of the automation workflow to ensure reliable and safe operation.

Software That Thinks Like a Chemist

Agilent's VnmrJ software 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 and easily.

Ease of Use

System design and validation is based on user workflows and typical day-to-day operations. Regardless of configuration, all of our advanced technology components fit together seamlessly to present each user with an easy-to-use, fully integrated system. This eliminates the need to reconfigure the system or use separate software for different workflows and use cases. New users appreciate the intuitive workflow design which shortens the learning curve.

Ease of ownership is built-in with automated maintenance and calibration tools to keep your system running at peak performance. Automated shimming has been elevated to an art in VnmrJ and is so good that you need never do manual shimming again. ProShim allows you to schedule or perform routine maintenance shimming and monitor system performance over time.
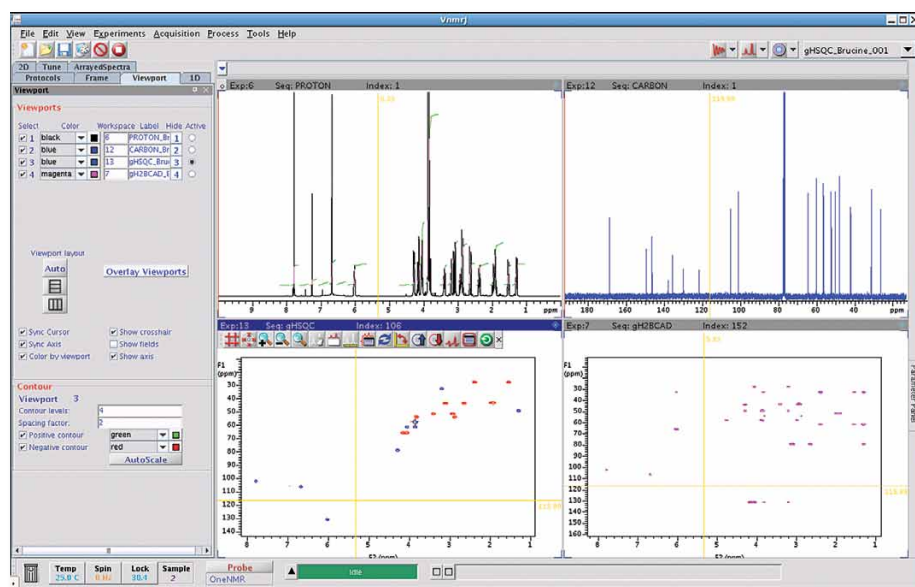
# PROBES: VERSATILITY AND PERFORMANCE

400 MHz OneNMR Probe

Versatility in a Single Probe

The OneNMR Probe represents the most significant advance in solution-state probe technology in over a decade. Simultaneously optimized for both high- and low-band frequencies, it delivers the performance advantages of both the classic carbon probe and the highly sensitive proton probe in a single design. But increased proton sensitivity is just one component of this new technology. The OneNMR Probe also provides outstanding RF homogeneity, excellent salt and solvent tolerance, improved water suppression, and superior lock sensitivity as compared to traditional probe technology.

The OneNMR Probe enables you to collect all of the data required for structure analysis of organic molecules, significantly reducing the labor and productivity loss associated with switching probes to conduct multiple experiments. Current users refer to it as "The Ultimate Routine Probe."

The OneNMR Probe delivers:

- A complete suite of experiments with no probe changes
- Minimal sample requirements due to high sensitivity on all frequencies
- Superior 1D and 2D performance through outstanding RF homogeneity and lock sensitivity
- High-quality NMR spectra due to outstanding line shapes
- ProbeID autonomous probe recognition and system configuration
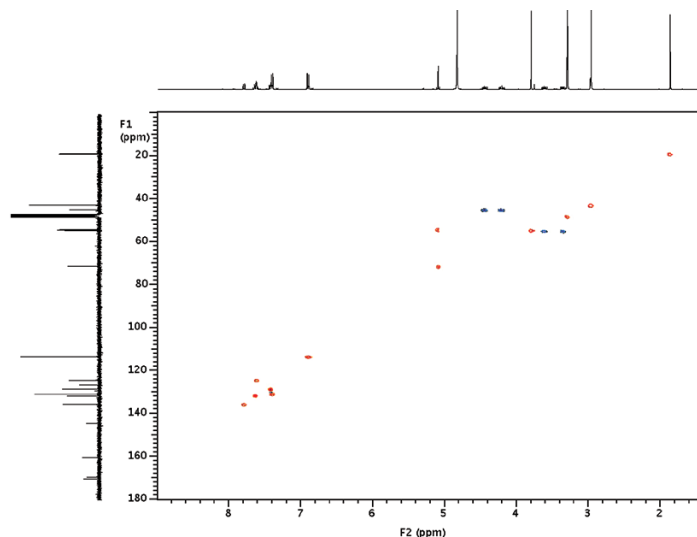
Superior 1D and 2D performance: HSQC spectrum of cis-diltazem collected on a 400-MR system equipped with a OneNMR Probe.

FLEXIBLE TOOLS FOR SAMPLE AUTOMATION

Agilent's suite of sample management tools increase system efficiency and enhance productivity by eliminating idle time between sample changes and extending the workday with unattended operation.

7620-AS Autosampler

The 7620-AS is simply the most advanced NMR autosampler available. It is a freestanding (vibration isolated) system capable of processing 96 samples in multiple modes. The robot manipulates the samples using the spinner turbine instead of the tube, enabling compatibility with a wide range of sample types. Sensors detect sample position and monitor key aspects of the automation workflow to ensure reliable and safe operation. In addition, industrial-scale robotics provide extended, maintenance-free operation. The 7620-AS also offers faster robot motion for improved throughput, an improved gripper arm and tube sensing for better sample handling, and seismic leg compatibility.

7510-AS Autosampler

The 7510-AS rotary autosampler provides maximum flexibility, operating in either batch or random access mode for up to twelve samples in spinners. This plug-and-play autosampler requires no adjustments; it features on-board sensors to monitor operation and is designed for extended maintenance-free operation.

Agilent NMR autosamplers were designed with your experiments in mind. Single-user, multi-user walkup, and high-throughput laboratories will all benefit from the combination of automation hardware and advanced VnmrJ software to organize, track, and manage the entire experimental workflow.


7620-AS autosampler (left) with close-up of robot handling sample (right).

7510-AS autosampler mounted on 400-MR magnet.

SOFTWARE THAT THINKS LIKE A CHEMIST

VnmrJ software is designed so that related NMR experiments can be organized and executed to quickly and efficiently deliver answers. A workflow-based structure where samples and their related data are paramount provides the flexibility to work the way you want. Take full control of the experiment or let the instrument do it automatically, it's your choice.

Agilent's intuitive operator interface allows for ultimate one-click flexibility. Packed with the latest pulse sequences, experimental protocols are readily located, collected and combined for effortless set-up and use. Moreover, results are fully accessible and easily manipulated to facilitate interactive data representation and analysis. Multiple experiments can be displayed on screen in parallel with coordinated tools such as cursors, zoom, and pan, enabling rapid and straightforward mining of peaks and contours that contain the chemical information you need. VnmrJ is also designed for automated handling of multiple samples from multiple chemists. Submitting sample information to the queue takes only seconds and results can be automatically sent to each chemist's computer.
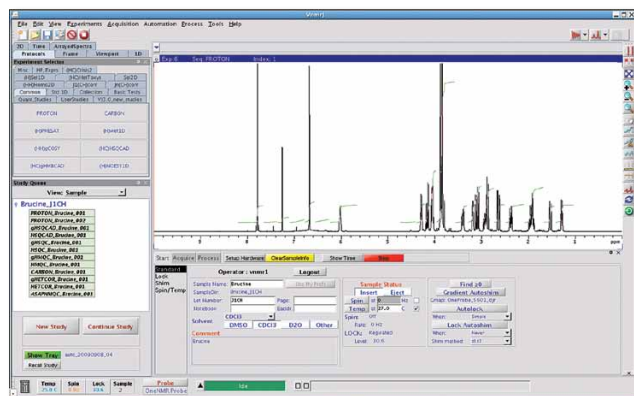
Key Features of VnmrJ Software

Setup and Experimental Design

- System utilities including Auto-Lock, Auto-Shim, Auto-Tune, and Auto-Calibration
- An extensive and up-to-date pulse sequence library for the best protocols
- One-click creation of new experiments, instantly available in Experiment Selector

Running Experiments

- Sample-centric data display and management
- Priority Sample queuing
- Extensive data analysis toolkit
- Automatic post-acquisition email of raw data and/or PDFs of your spectrum
- ProShim for advanced automatic shimming
- One-click absolute quantitative analysis
- Adaptive NMR – intelligent autonomous experiment optimization

VnmrJ was also designed with the administrator in mind. In addition to capabilities such as automatic calibration, automatic shimming, and remote system monitoring that are requisite for efficient high-throughput operation, the software package includes spreadsheet-based sample submission for batch runs and data mirroring to ensure data integrity and system security.

# 400-MR SPECTROMETER PROVEN CONSOLE ARCHITECTURE

Console Architecture

The 400-MR'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. In addition, advanced phase and amplitude modulation offer exceptional performance for automated "fast" liquids experiments. The DD2 console was redesigned for improved performance and ease-of-use, and now incorporates VT (variable temperature) support in the standard console.

NMR Magnets

The 400-MR's Premium Shielded NMR magnet performs in a wide range of work environments. The small fringe field, robust interference attenuation, and anti-vibration support legs add up to a system that adapts to a variety of locations with minimal site preparation. The long cryogen hold time minimizes maintenance and high field homogeneity ensures excellent data quality.

Agilent's DirectDigital receiver provides greater accuracy, better signal-to-noise, and cleaner spectra, ensuring confidence in the quantitation of minor impurity peaks, such as the one highlighted here.
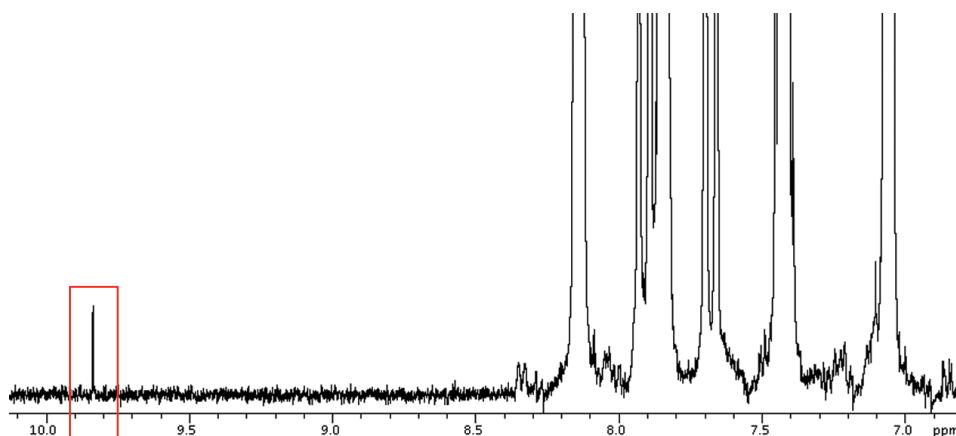
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