The OneNMR Probe for Routine Chemical Applications

Technical Overview

Advantage Statement

In the past, sophisticated NMR users needing data on a small-molecule sample either used several NMR probes, each optimized for a different type of experiment, or they compromised on performance by selecting a single probe solution for all of their studies. With the introduction of the Agilent OneNMR Probe, ALL users can now achieve outstanding performance for ALL of their experiments without the need to ever change a probe.

The OneNMR Probe combines the ^{13}C performance features of the classic carbon probe (used for direct-observed, heteronuclear data) with the extraordinary ^{1}H sensitivity and lineshape of a dedicated proton probe (used for the acquisition of indirect-observed NMR data). The Agilent OneNMR Probe offers the simplest day-to-day operation for a routine NMR system while delivering uncompromised results. The OneNMR Probe is truly a one-probe solution for routine organic chemistry applications.

Agilent Technologies

OneNMR Probe Performance Specifications

Feature	Benefit
Outstanding lineshape simultaneously on both frequency channels ^{1}H < 0.8/7.0/14 non-spinning ^{13}C < 0.2/3.0/5.0 spinning	The highest quality NMR spectra available on both frequency channels
Excellent sensitivity on all frequencies (^{1}H, ^{19}F, ^{2}H, and ^{31}P to ^{15}N) ^{1}H > 650:1, ^{13}C > 220:1	A minimum of sample is required to obtain high-quality NMR spectra
Unmatched B_1 field homogeneity ^{1}H 810/90 = 70%	Use of the most demanding pulse sequences with maximum recovery of the available sensitivity
Short 90 degree pulse widths on both frequency channels ^{1}H 90 degree pulse < 8 µsec ^{13}C 90 degree pulse < 10 µsec	Uniform excitation across the broadest possible frequency window

These performance characteristics match those of the best indirect-detection and broadband probes available and combine to generate exceptional small molecule NMR data, as shown in Figure 1.

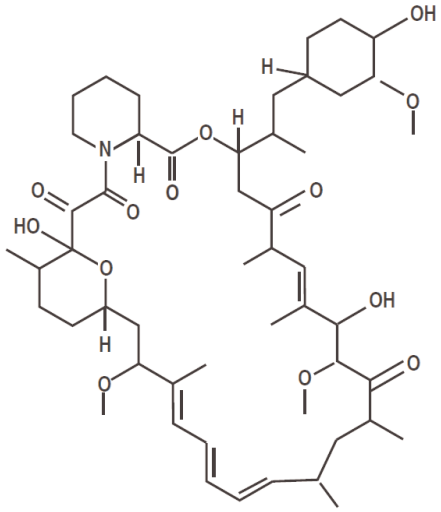
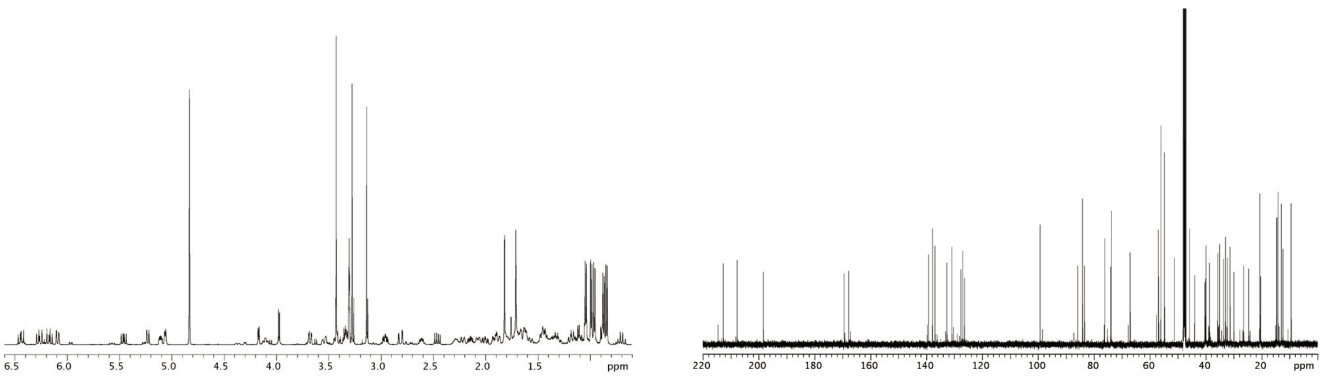
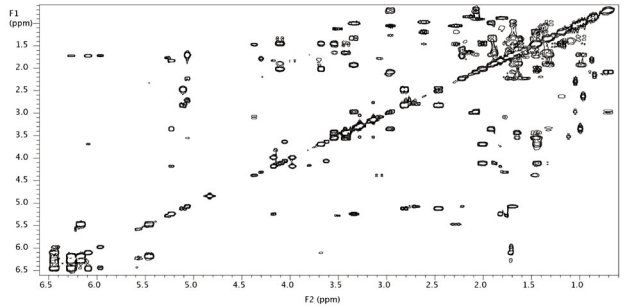


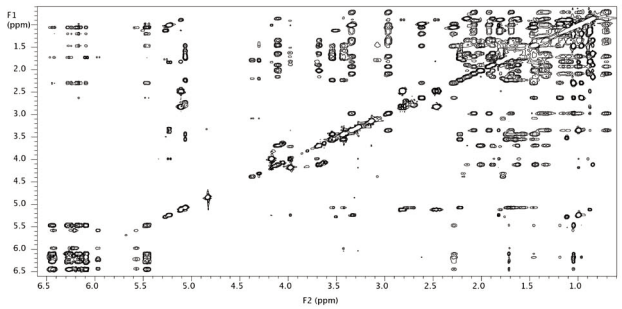
Figure 1. Structure of rapamycin.



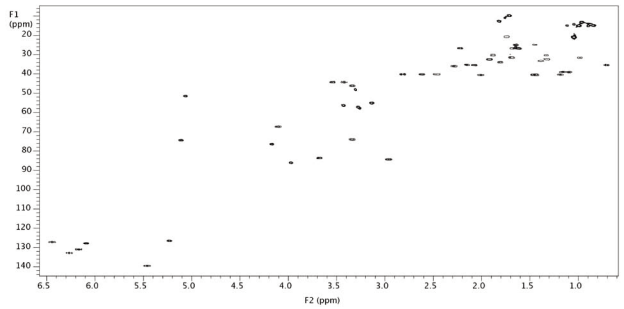
OneNMR Probe ^{1}D 1H and ^{13}C NMR Spectra of Rapamycin. This marketed immunosuppressive agent displays complex NMR spectra with highly congested aliphatic regions and resonances due to a minor conformer visible across the entire spectral window in both data sets. The superb resolution of the OneNMR Probe retains the maximum available dispersion and minimizes spectral overlap, thereby simplifying interpretation of the data. Best of all, since the OneNMR Probe is simultaneously optimized on both the high-band and low-band frequencies, it requires no probe changes for full intensity 1D-proton and 1D-carbon spectra.



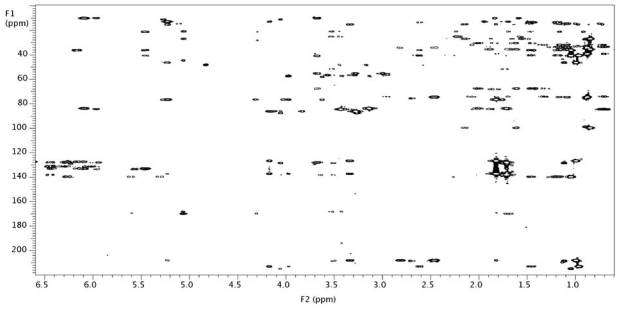
OneNMR Probe COSY Spectrum of Rapamycin. This homonuclear correlation experiment is the mainstay of 2D homonuclear NMR spectroscopy. The OneNMR Probe generates these types of data with ease even on mass-limited samples.



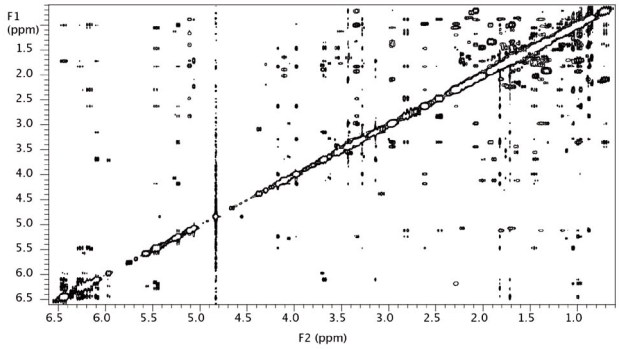
OneNMR Probe TOCSY Spectrum of Rapamycin. This homonuclear correlation data set is used to map proton coupling pathways across multiple bonds. The high B_1 field homogeneity of the OneNMR Probe allows TOCSY data to be acquired with minimal loss in sensitivity due to probe effects.



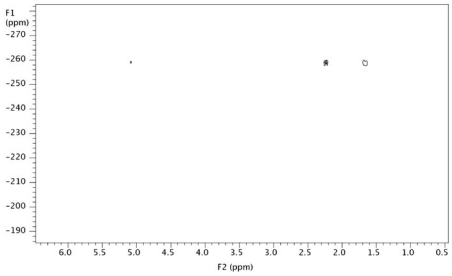
OneNMR Probe Multiplicity-Edited HSQC Spectrum of Rapamycin. The HSQC data set has become a cornerstone of small-molecule NMR spectroscopy for structure elucidation problems. The unmatched simultaneous performance of the OneNMR Probe on the proton and carbon channels allows one to collect spectacular HSQC spectra without the need to change probes.



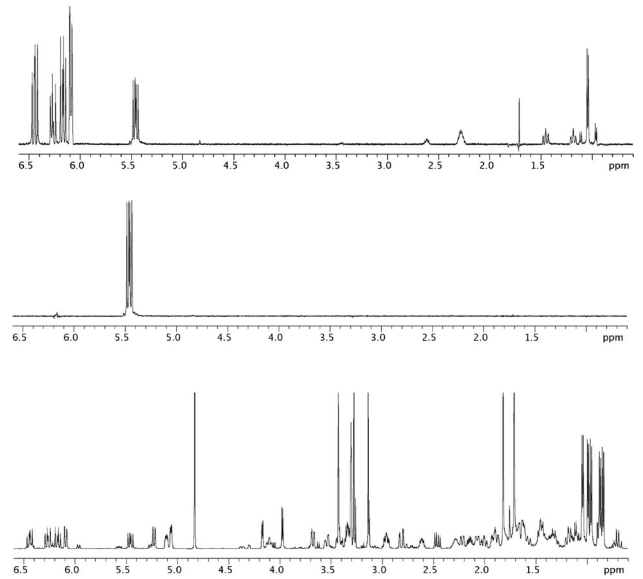
OneNMR Probe HMBC Spectrum of Rapamycin. The HMBC experiment is a comparatively low-sensitivity experiment and is therefore demanding of the entire NMR system. Good HMBC performance requires crisp, accurate pulses on the ^{13}C channel and excellent proton sensitivity. By combining the ^{13}C pulse performance of a broadband probe with the ^{1}H spectral quality of an indirect probe, the OneNMR Probe represents the ultimate probe design for HMBC data collection.



OneNMR Probe NOESY Spectrum of Rapamycin. The NOESY experiment provides information on through-space interactions and is routinely used to answer questions in the structural chemistry setting. Even the strongest NOESY responses in a typical organic molecule are relatively small, which means that the superior sensitivity of the OneNMR Probe provides a tremendous advantage for this experiment (as compared to the types of probes typically employed for routine applications).



OneNMR Probe ^{1}H-^{15}N HMBC Spectrum of Rapamycin. Proton-nitrogen correlation data can be a powerful tool for structure elucidation, but acquisition of the data is challenging due to the large chemical shift window of the ^{15}N nuclide. The OneNMR Probe offers much shorter heteronuclear pulse widths on nitrogen than a conventional inverse probe, which moves this difficult experiment into the realm of routine NMR.



OneNMR Probe 1D TOCSY Spectrum of Rapamycin, showing the reference spectrum (bottom), the excitation profile (middle), and the spinlock result (top). The 1D TOCSY experiment allows visualization of complete spin systems without interference from overlapping resonances. The OneNMR Probe performs these experiments with ease.

www.agilent.com

Printed in the USA
March 25, 2011
SI-1477

Agilent Technologies