

# Fast, Effective Lineshape Optimization on the Agilent 400-MR

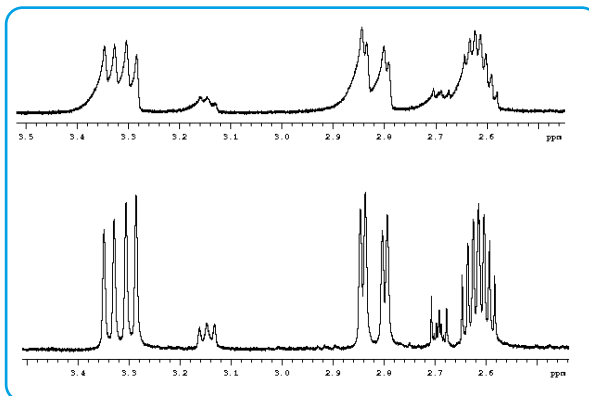
## Data Sheet

### Introduction

Agilent's 400-MR uses rapid gradient shimming methods to optimize lineshape prior to data acquisition. This technique, typically run automatically, provides improved sensitivity and data quality for organic and inorganic molecules in a variety of solvents, including DMSO-d<sub>6</sub>, D<sub>2</sub>O, H<sub>2</sub>O, C<sub>6</sub>D<sub>6</sub>, and CDCl<sub>3</sub>.

### Key Benefits

- **Sensitivity**—Increased information content. Narrower lines improve signal intensity. The optimal lineshape provides greater spectral fine structure.
- **Easy to use**—Gradient shimming operates as part of the experiment protocol.
- **Fast**—Gradient shimming is up to 4 times faster than alternative simplex algorithm techniques.
- **Robust and reliable**—Unlike simplex routines, gradient shimming is insensitive to local minima.
- **Always available**—Gradient shimming can be run on any combination of spectrometer, probe and software.



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## Gradient Shimming Methods

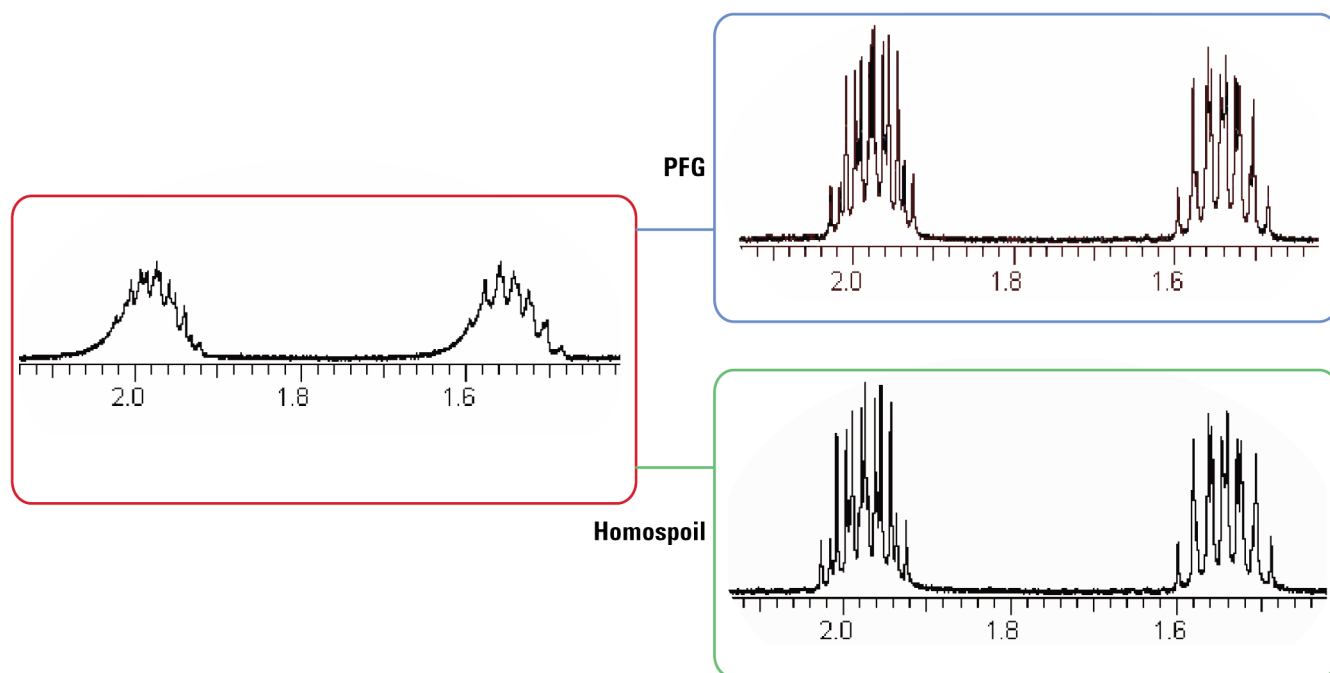
Gradient shimming on the Agilent 400-MR can be achieved using two different methods. For probes that contain a Pulsed Field Gradient (PFG) coil, such as the Automated Triple Broadband (ATB), AutoSwitchable (ASW) and AutoTune probes, field profiles can be generated with the PFG hardware that is provided standard with every 400-MR. For probes that do not have a PFG coil, such as the 10-mm broadband probe, the field profiles can be generated with homospoil gradients generated with the room temperature shim coils which are located between the probe and the magnet. The spectra resulting from either method are of equal quality.

## Proton or Deuterium Gradient Shimming Available

Gradient shimming can be run on the protons in a sample or the deuteriums in a sample, either of which are usually the solvent, but can also be other sample components.

### Applications Include:

- Organic synthesis confirmation
- Rapid reaction mixture analyses
- Urine or other biofluid samples in water



**Figure 1**

Starting from the same unshimmed state (left), data from a sample of ethylindanone in  $\text{CDCl}_3$  was acquired with an Agilent 400-MR using automatic PFG gradient shimming (top right) and homospoil gradient shimming (bottom right). In both cases, the shimming process took less than 1 minute. The results are essentially identical.

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