PURE SHIFT NMR METHODS

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Homonuclear spin-spin couplings are simultaneously a great strength and a great weakness of NMR spectroscopy. A great strength because of the wealth of information they convey about chemical structure and stereochemistry, and a great weakness because the multiplet structure they cause greatly increases the frequency width of the NMR signals for a given chemical site. Multiplet structure is a particular challenge in ^{1}H NMR because of the narrow (*ca*. 10 ppm) range of typical ^{1}H chemical shifts, which means that all but the simplest species show spectra in which the multiplet signals from different chemical sites overlap. From the early days of ^{1}H NMR it was recognized[1] that it would be immensely useful to be able to switch off the effects of homonuclear couplings, as it subsequently became possible to do for heteronuclear couplings with broadband decoupling, to give a ^{1}H spectrum with just one peak per chemical site – a "pure shift" spectrum (see Figure 1). Over the last 20 years a series of developments[2-4] have made it possible to approach this ideal very closely, improving the resolution of ^{1}H NMR by almost an order of magnitude. This tutorial lecture will describe the development of pure shift NMR methods, survey the current state of the art, and show some applications.

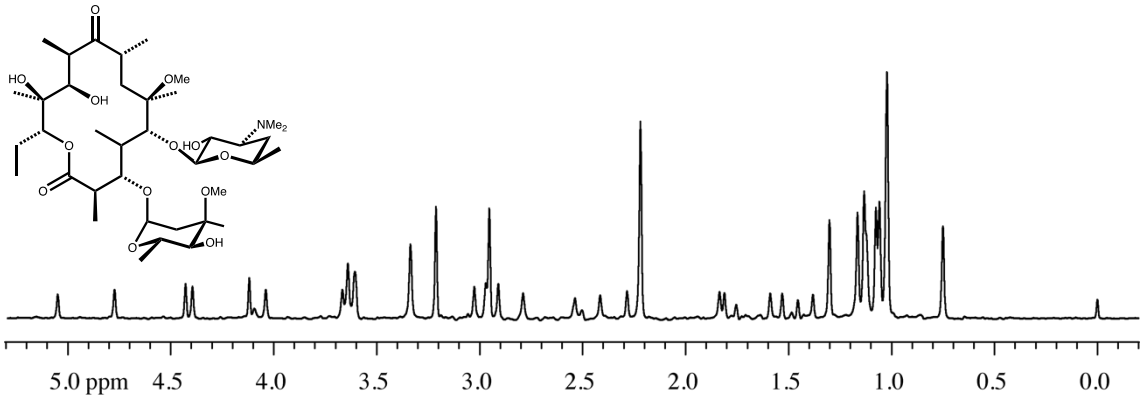

Figure 1. 500 MHz ^{1}H NMR spectrum of the antibiotic clarithromycin.

Acknowledgements. This work has been supported by the Engineering and Physical Sciences Research Council.

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