Erythromycin A

Erythromycin A is a broad-spectrum, macrolide antibiotic on the World Health Organization's List of Essential Medicines. It is often used for the treatment of a wide variety of bacterial infections including respiratory tract infections, skin infections, pelvic inflammatory disease. Figure 1 shows the 1H NMR spectrum of a 90 mM Erythromycin A sample in $CDCl_3$ measured in a single scan taking 10 seconds to acquire.

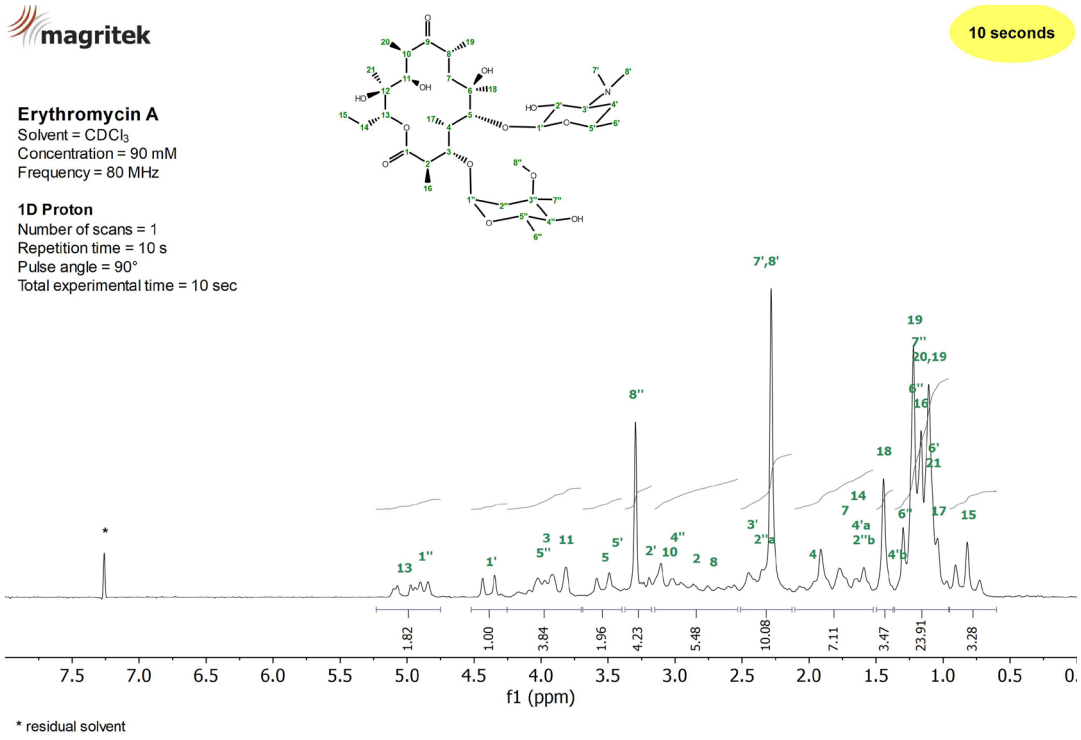

Figure 1: ^{1}H NMR spectrum of a 90 mM Erythromycin A sample in $CDCl_3$ measured on a Spinsolve 80 MHz ULTRA system in a single scan.

^{13}C Spectrum

Figure 3 shows the ^{13}C NMR spectrum of 90 mM Erythromycin A in $CDCl_3$ acquired using NOE polarization transfer from ^{1}H to ^{13}C and ^{1}H decoupling. The 1D Carbon experiment using NOE is sensitive to all ^{13}C nuclei in the sample. It clearly resolves all the expected resonances.

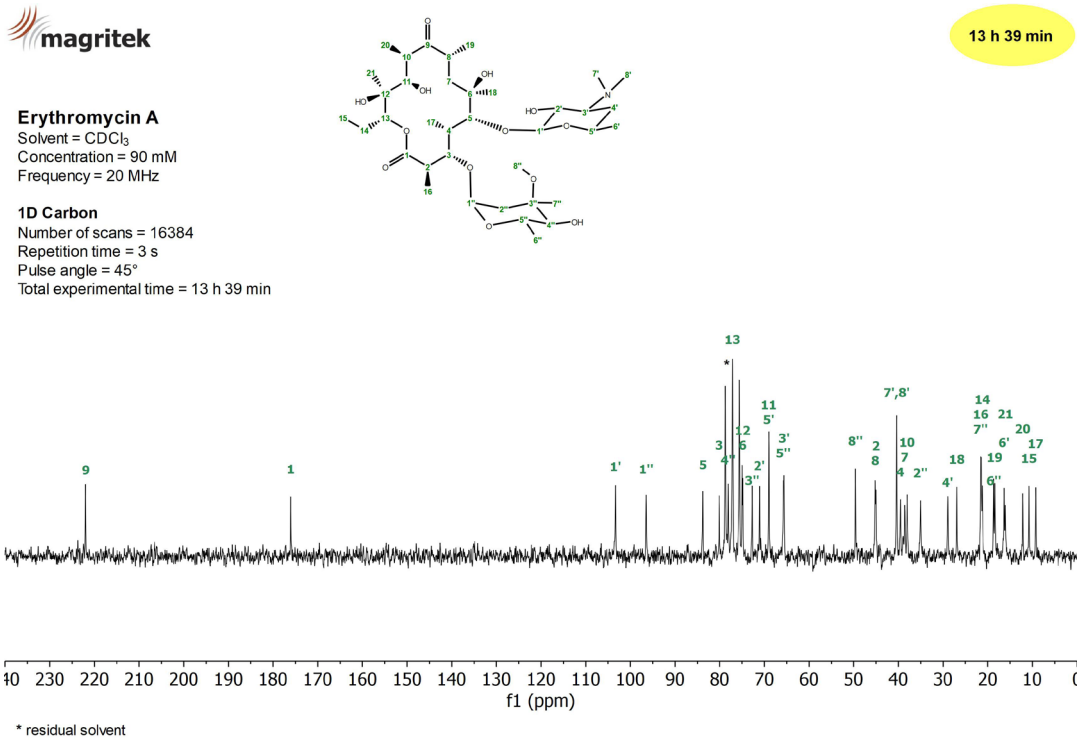

Figure 2: ^{13}C NMR spectrum of a 90 mM Erythromycin A sample in $CDCl_3$ measured on a Spinsolve 80 MHz ULTRA system in 13 h 39 minutes.

2D COSY

The 2D COSY experiment allows one to identify coupled ^{1}H nuclei as they generate cross peaks out of the diagonal of the 2D data set. In Figure 3 a large number of cross peaks can be nicely observed. For example, the proton at position 1" couples to protons 2" (orange); and the proton 1' couples with proton 2' (light green). The proton 3 couples with proton 2 (dark green) and proton 4 (red). The proton 4 also couples to proton 5 (blue). In addition, the coupling between protons 14 and 15 (pink) can be observed.

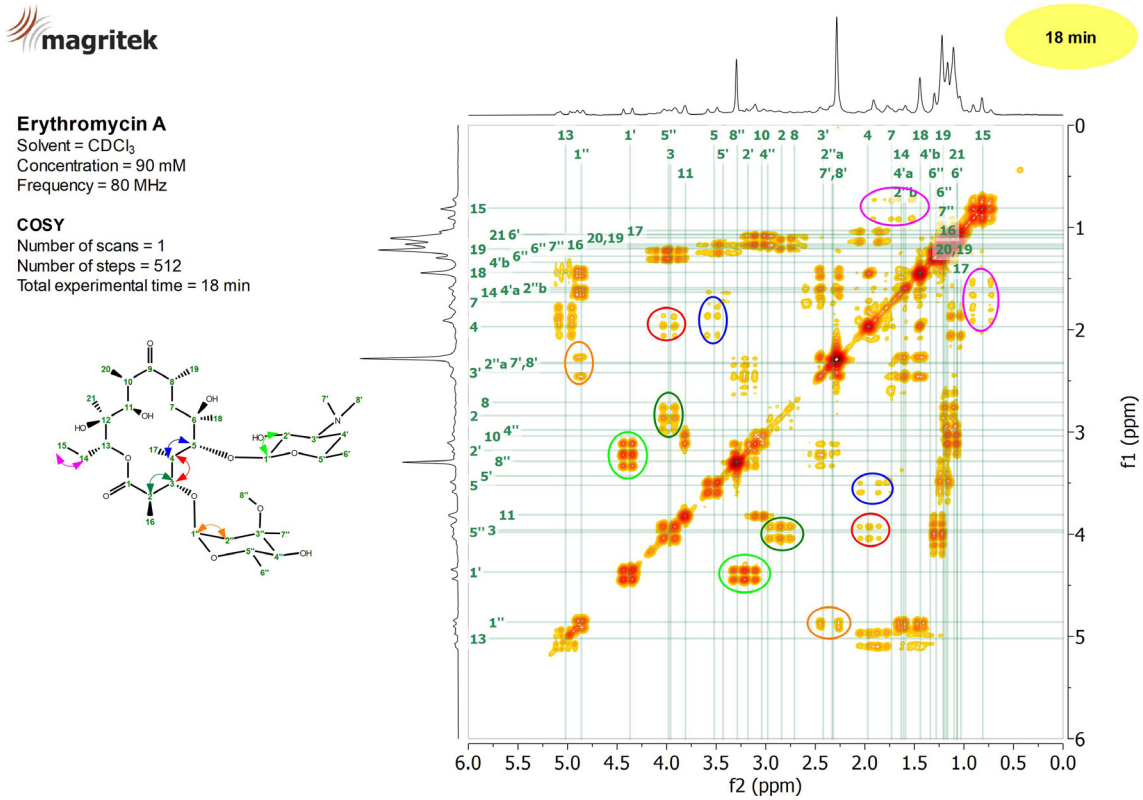

Figure 3: ^{1}H 2D COSY experiment of a 90 mM Erythromycin A sample in $CDCl_3$ acquired in 18 minutes on a Spinsolve 80 MHz ULTRA system.

2D J-Res

The 2D J-Res experiment is useful to identify the chemical groups generating a single line for each group by collapsing the J-coupling along the direct direction. The multiplets are generated along the vertical direction.

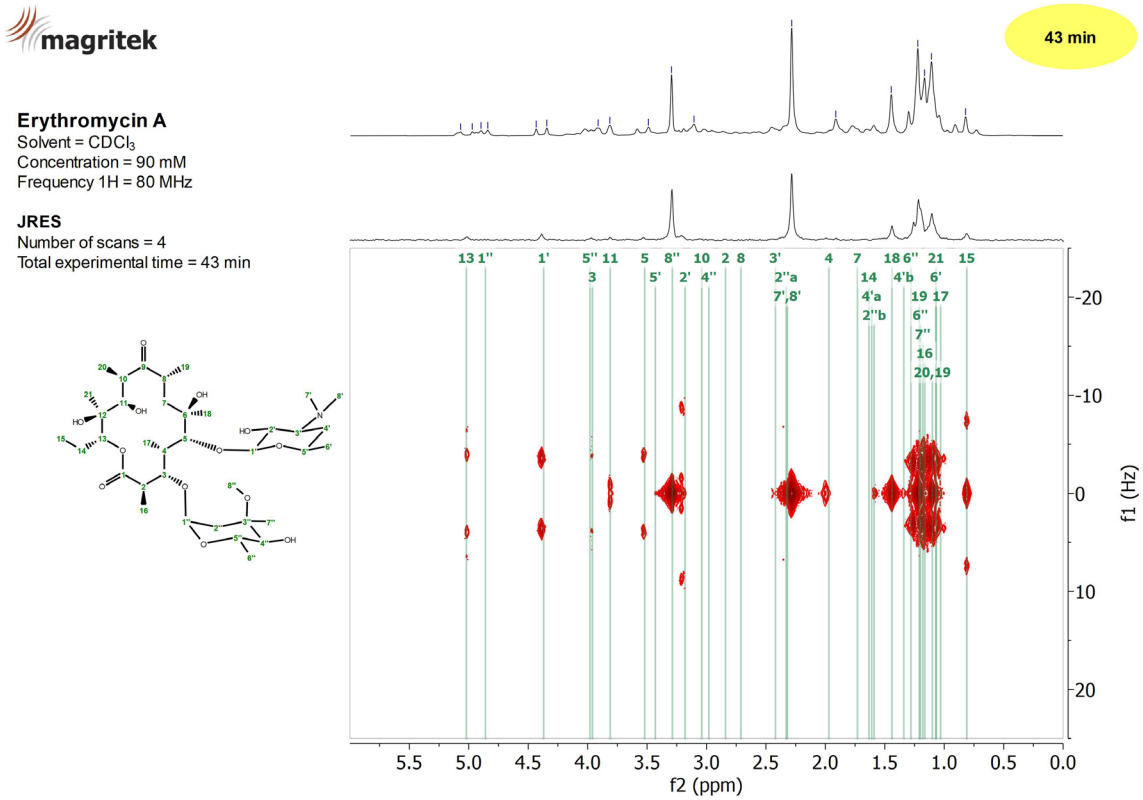

Figure 4: ^{1}H 2D J-Res experiment of a 90 mM Erythromycin A sample in $CDCl_3$ acquired in 43 minutes on a Spinsolve 80 MHz ULTRA system.

2D HSQC-ME

The HSQC is a powerful sequence widely used to correlate ^{1}H with the one-bond coupled ^{13}C nuclei. The Spinsolve is equipped with a multiplicity edited version (HSQC-ME) of this method. It provides the editing power of the DEPT-135 sequence, which is useful to differentiate the signals of CH_2 groups (blue) from CH and CH_3 groups (red). Figure 5 shows the HSQC-ME spectrum of a 90 mM Erythromycin A in $CDCl_3$ acquired in 137 minutes.

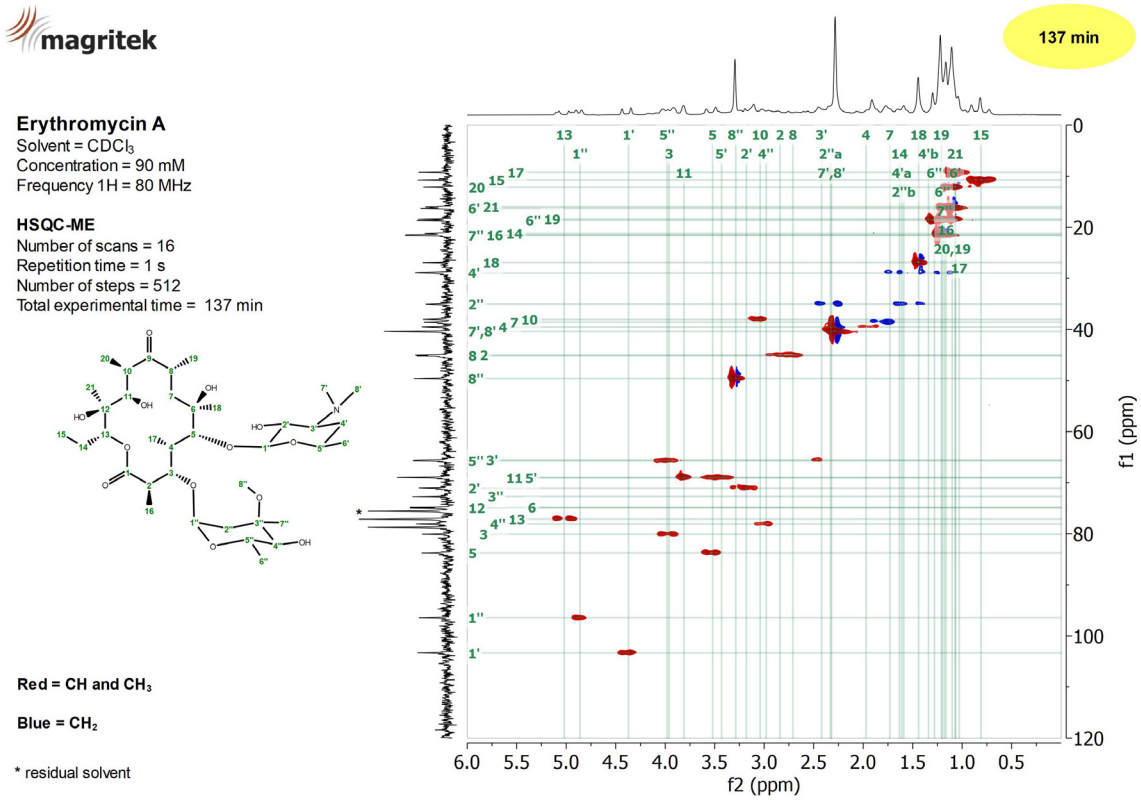

Figure 5: HSQC-ME spectrum of a 90 mM Erythromycin A sample in $CDCl_3$ showing the correlation between ^{1}H and ^{13}C signals.

2D HMBC

To obtain long-range ^{1}H -^{13}C correlations through two or three bond couplings, the Heteronuclear Multiple Bond Correlation (HMBC) experiment can be used. Figure 6 shows the HMBC spectrum of a 90 mM Erythromycin A sample in $CDCl_3$ measured in 274 minutes on our Spinsolve 80 MHz ULTRA. As an example, the long-range correlations of quaternary carbon 9 with protons 11 (orange), 10 (blue) and 7 (light green) are marked with circles.

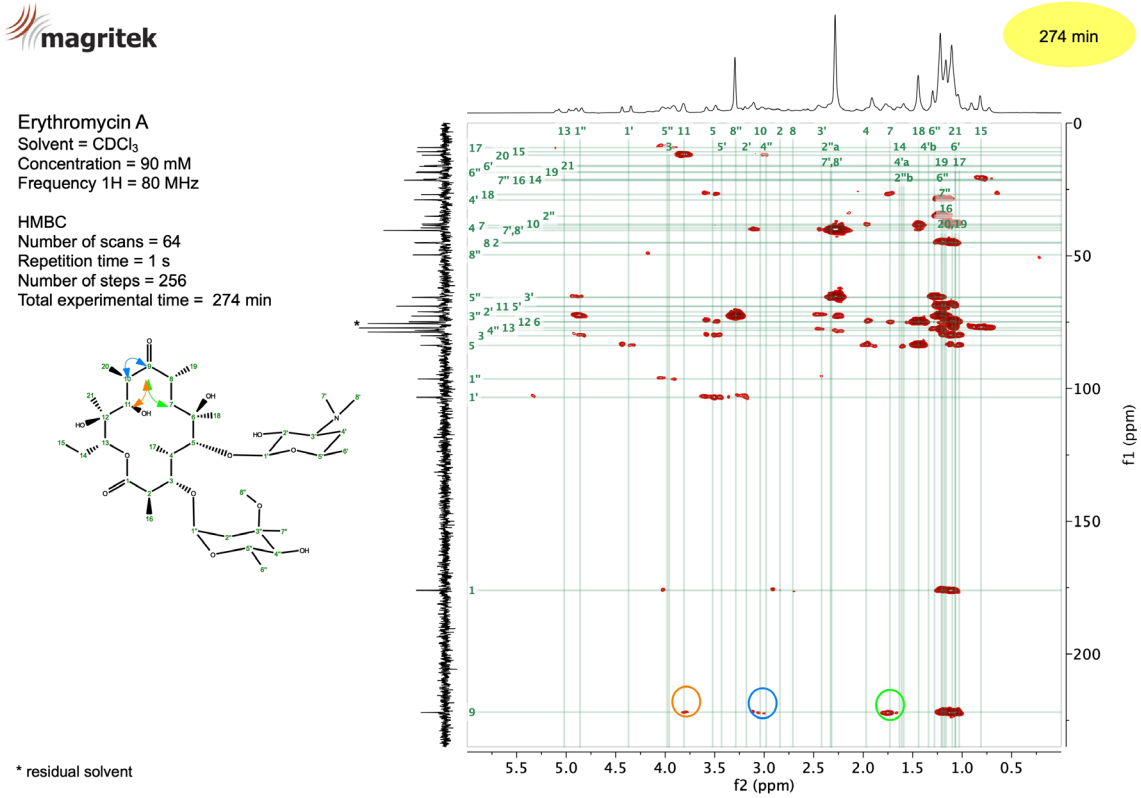

Figure 6: HMBC spectrum of a 90 mM Erythromycin A sample in $CDCl_3$ showing the long-range couplings between ^{1}H and ^{13}C nuclei.