Quinine

Spinsolve™ 60

Quinine is a drug used to treat a variety of conditions, most notably malaria. It is listed as one of the WHO's (World Health Organization's) "Essential Medicines". Figure 1 shows the ^{1}H NMR spectrum of 250 mM Quinine in $CDCl_3$ measured in a single scan taking 10 seconds to acquire.

1D Proton spectrum

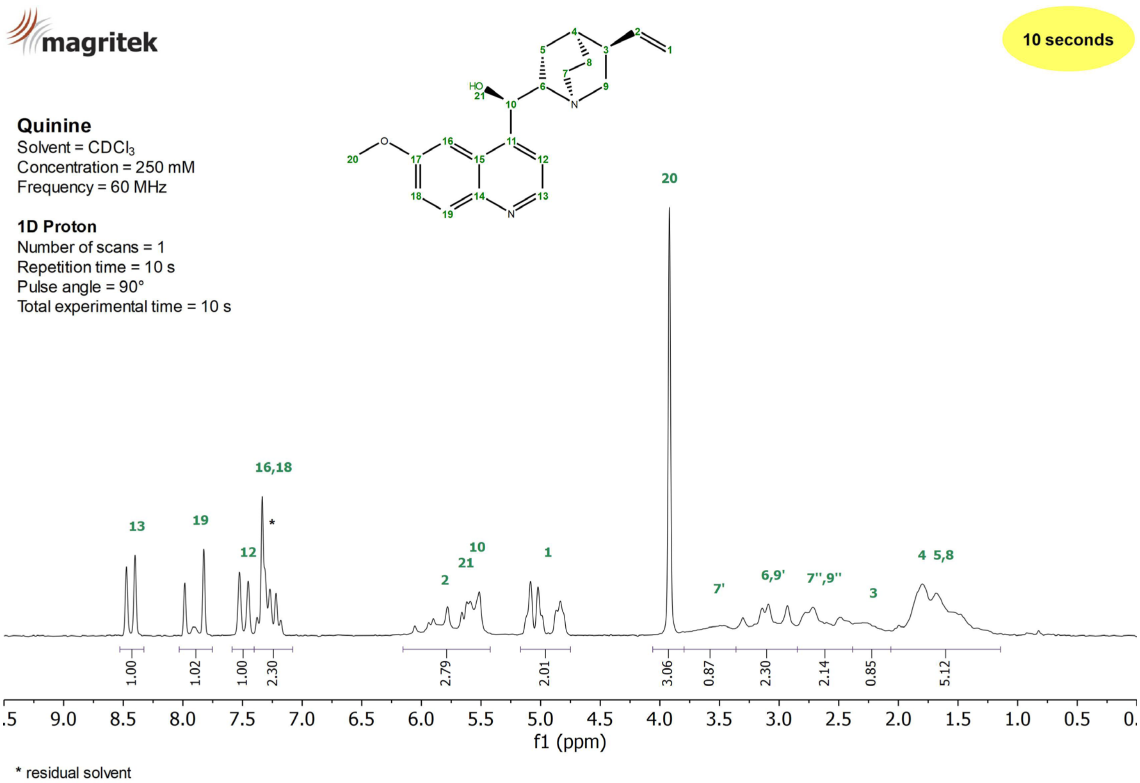

Figure 1: ^{1}H NMR spectrum of 250 mM Quinine in $CDCl_3$ measured on a Spinsolve 60 MHz system in a single scan.

1D Carbon spectrum

Figure 2 shows the ^{13}C NMR spectrum of 250 mM Quinine 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.

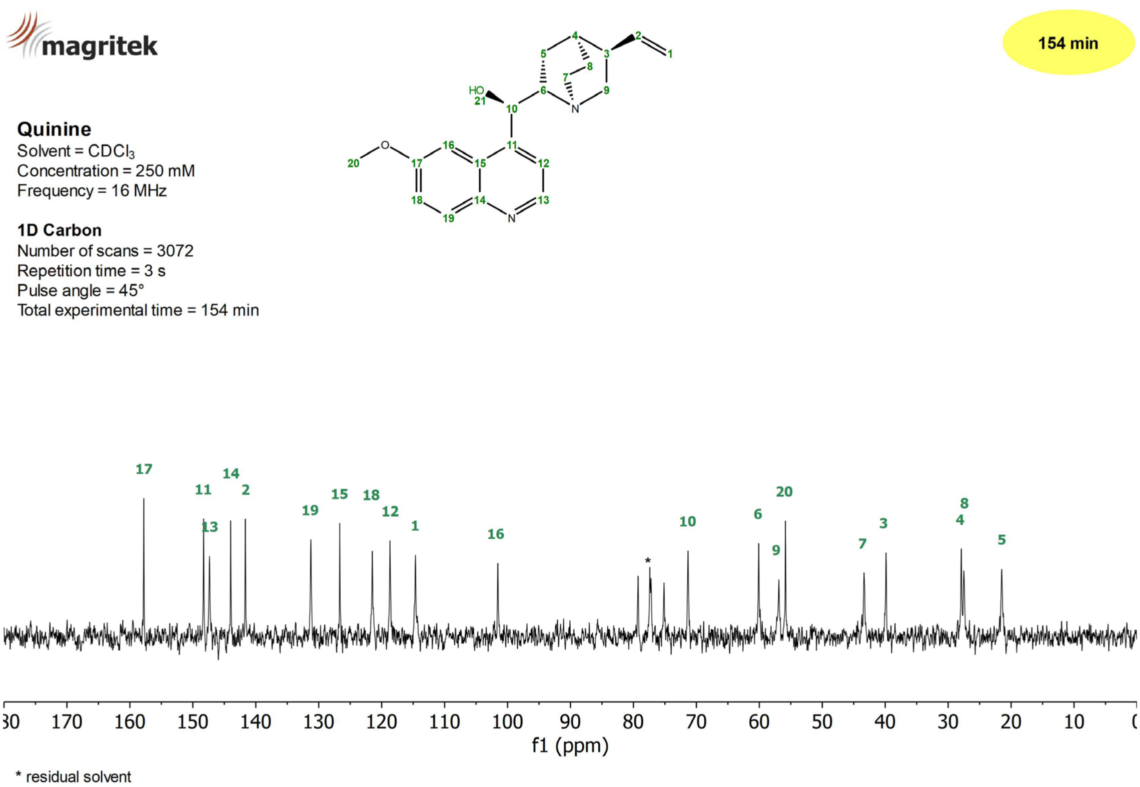

Figure 2: ^{13}C NMR spectrum of 250 mM Quinine in $CDCl_3$ measured on a Spinsolve 60 MHz system in 154 minutes.

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2D COSY spectrum

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 observed nicely. For example, the proton at position 13 couples to proton 12 (dark blue), the protons 16 and 18 couple to protons 20 (orange), proton 18 couples to proton 19 (light green), proton 2 couples with protons 1 (pink) and proton 3 (light blue). In addition, the coupling between protons 3 and 9 (dark green) and protons 6 and 10 (red) can be observed.

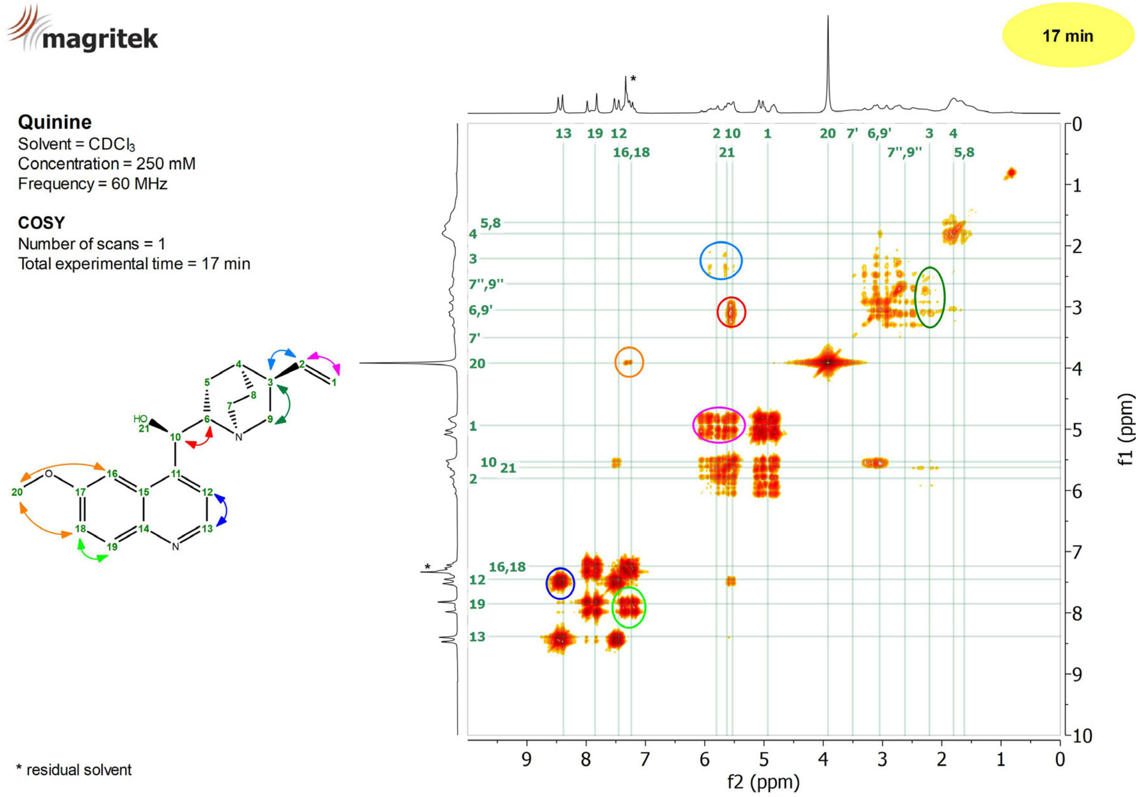

Figure 3: ^{1}H 2D COSY experiment of 250 mM Quinine in $CDCl_3$ acquired in 17 minutes on a Spinsolve 60 MHz system.

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 4 shows the HSQC-ME spectrum of 250 mM Quinine in $CDCl_3$ acquired in 8 minutes.

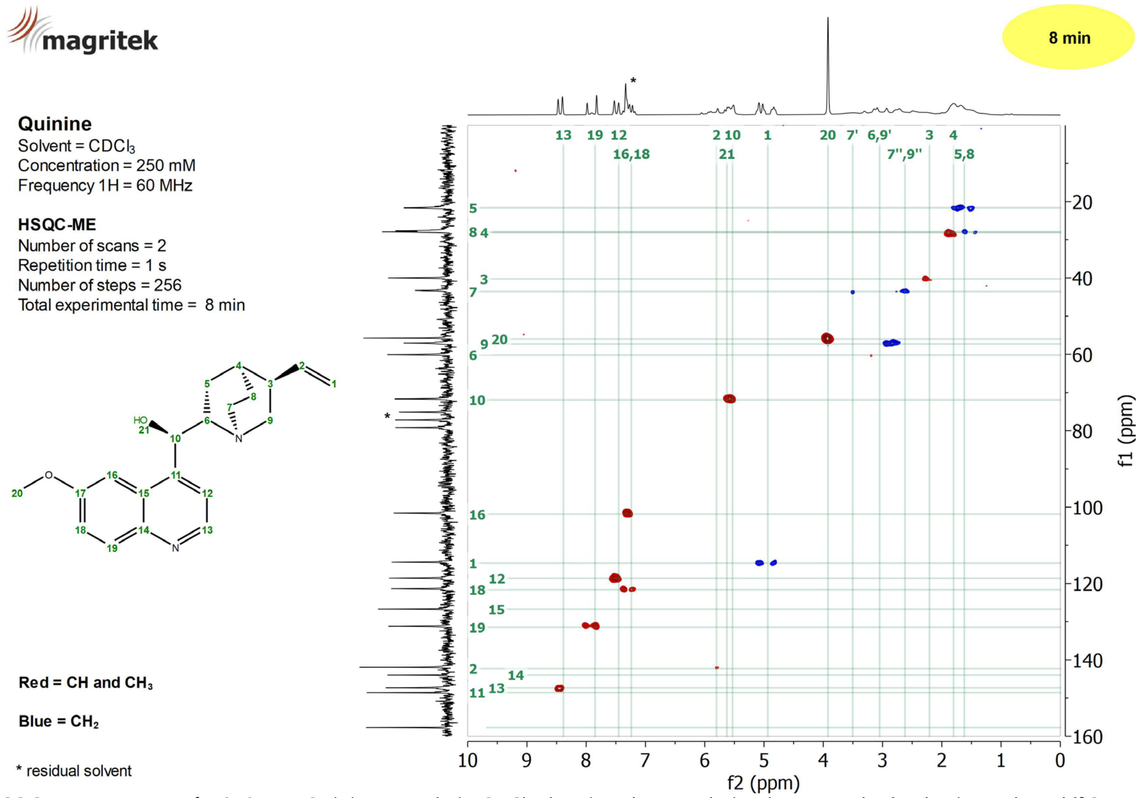

Figure 4: HSQC-ME spectrum of a 250 mM Quinine sample in $CDCl_3$ showing the correlation between the ^{1}H (horizontal) and ^{13}C (vertical) signals.

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 5 shows the HMBC spectrum of a 250 mM Quinine sample measured in 69 minutes on our Spinsolve 60 MHz. As an example, the long-range correlations of proton 13 with carbons 12 (dark blue), 14 (light green) and 11 (red), as well as the couplings of proton 19 with carbons 15 (light blue) and 17 (pink), the coupling of proton 12 with carbon 10 (orange) and protons 20 with carbon 17 (dark green) are marked with circles. The experiment shows the correlation with quaternary carbons, too.

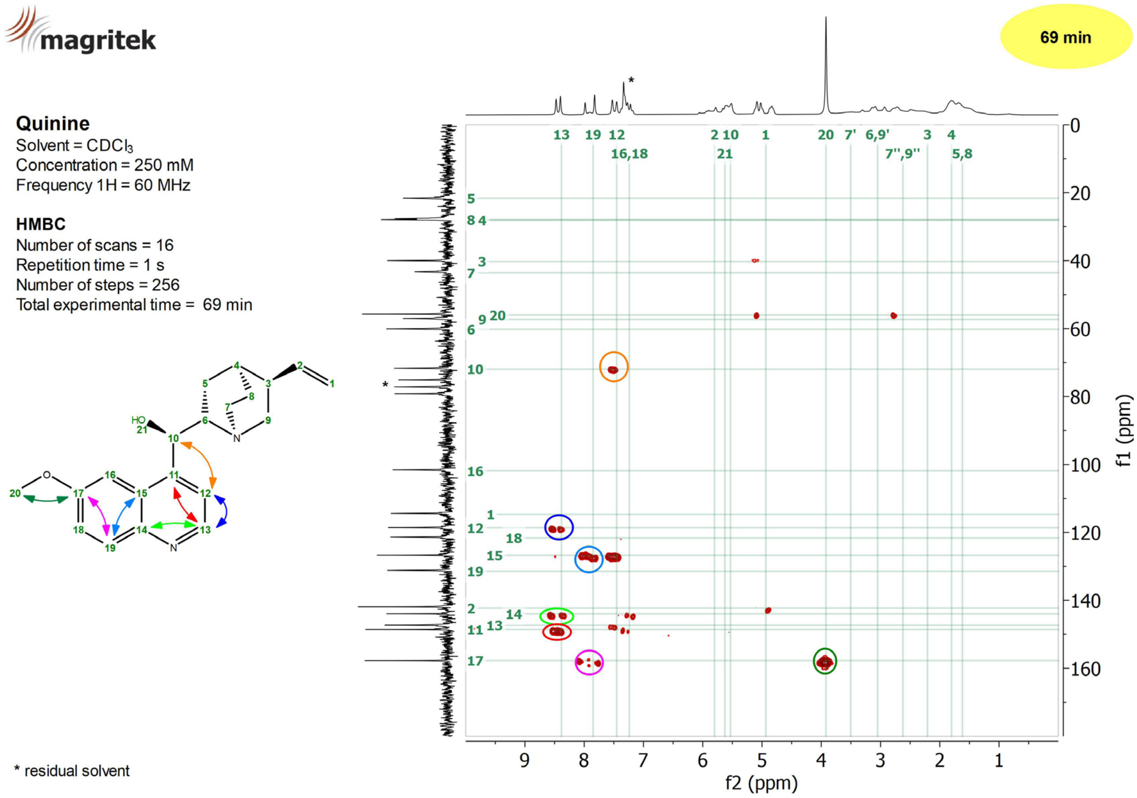

Figure 5: HMBC spectrum of a 250 mM Quinine sample in $CDCl_3$ showing the long-range couplings between ^{1}H and ^{13}C nuclei.