Artemisinin

Spinsolve™ 60

Artemisinin is a widely used drug in the standard treatment of malaria. It is extracted from the plant *Artemisia annua*, sweet wormwood, but can also be produced in a semi-synthetic fashion. Figure 1 shows the ^{1}H NMR spectrum of a 250 mM Artemisinin sample in $CDCl_3$ measured in a single scan taking 10 seconds to acquire.

1D Proton spectrum

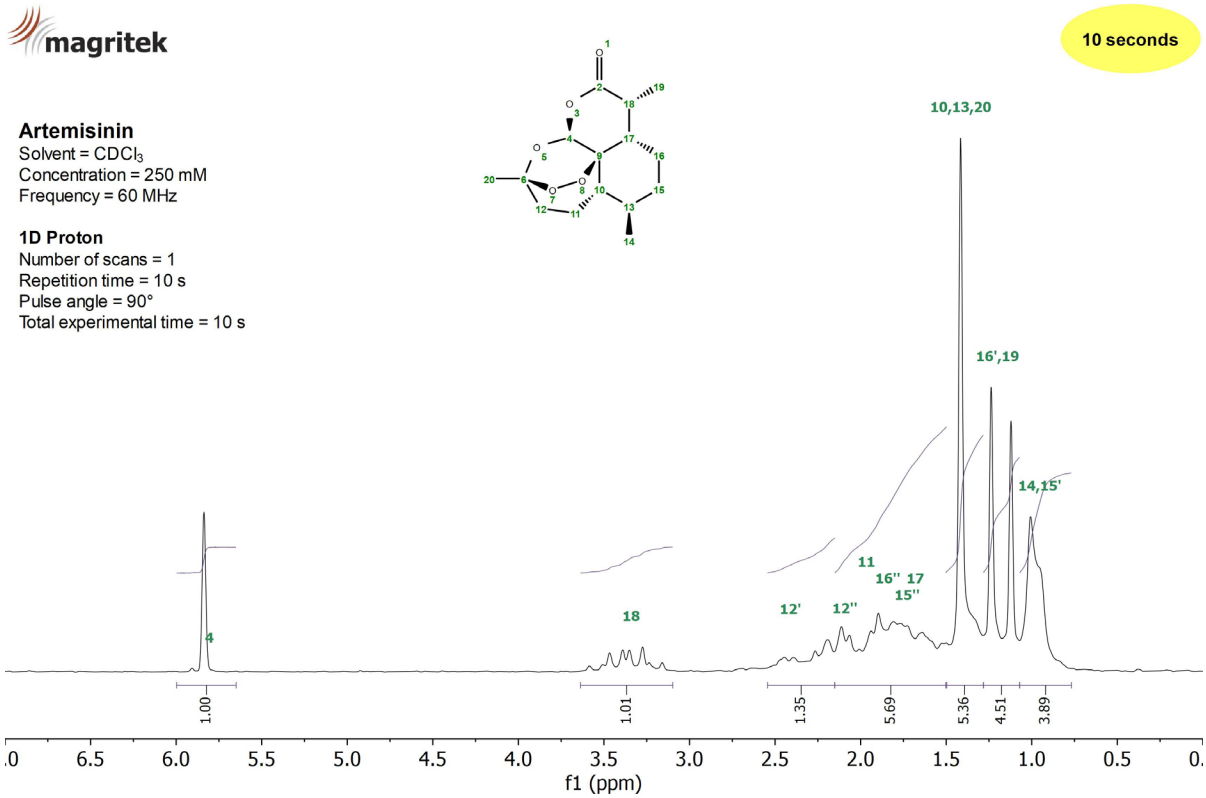

Figure 1: ^{1}H NMR spectrum of a 250 mM Artemisinin sample in $CDCl_3$ measured on a Spinsolve 60 MHz system in a single scan.

1D Carbon spectrum

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

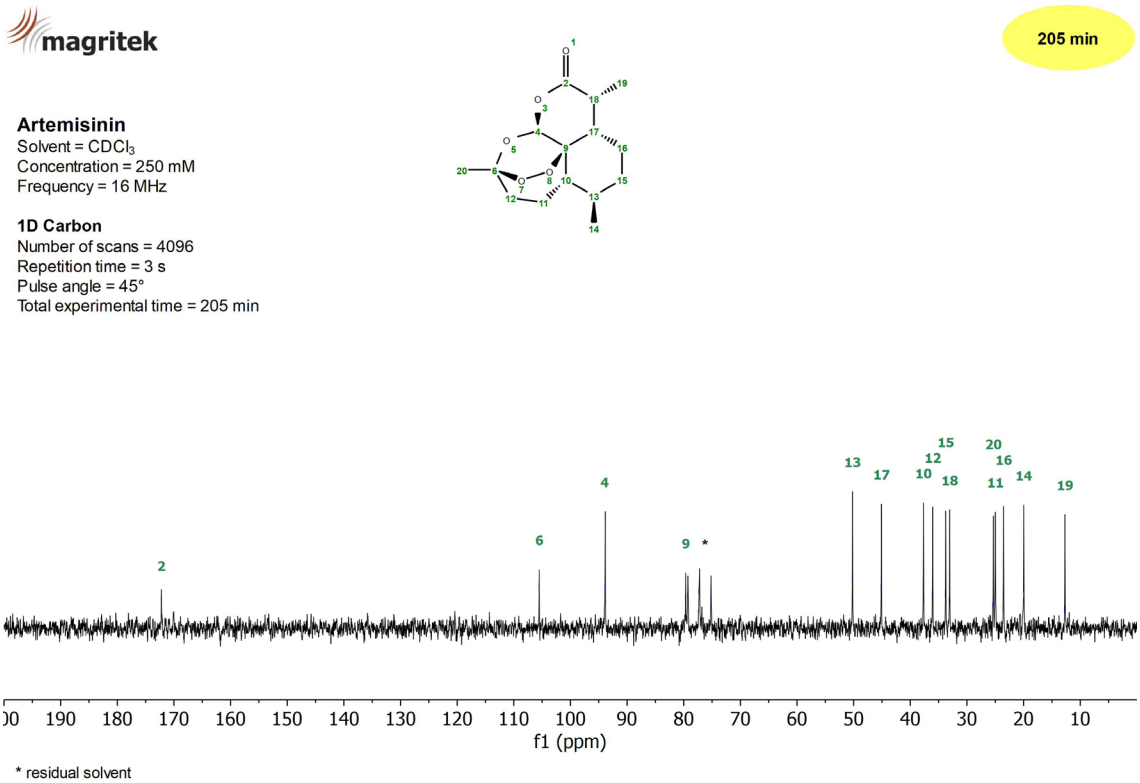

Figure 2: ^{13}C NMR spectrum of a 250 mM Artemisinin sample in $CDCl_3$ measured on a Spinsolve 60 MHz system in 205 minutes.

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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 nicely observed. For example, the protons at position 4 and 17 (dark blue) couple with each other. Furthermore, proton 18 couples with proton 17 (cyan) and 19 (pink).

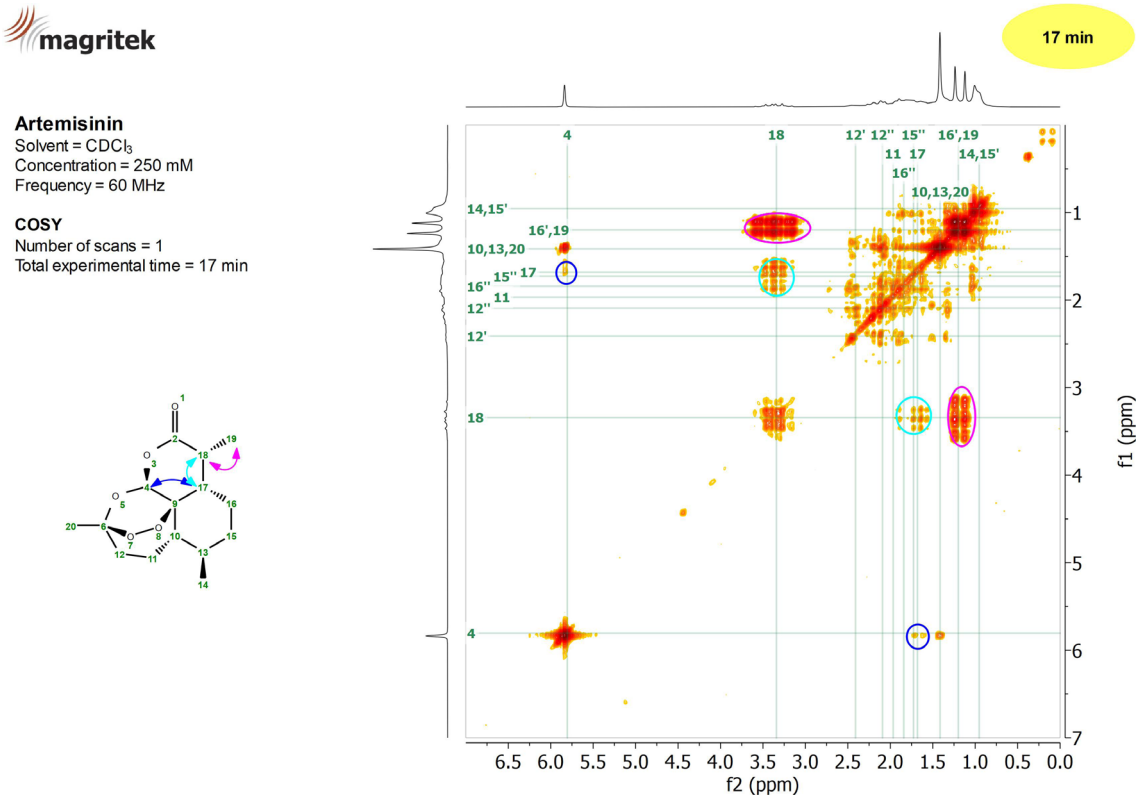

Figure 3: ^{1}H 2D COSY experiment of a 250 mM Artemisinin sample in $CDCl_3$ acquired in 17 minutes on a Spinsolve 60 MHz system.

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 a 250 mM Artemisinin sample in $CDCl_3$ acquired in 34 minutes.

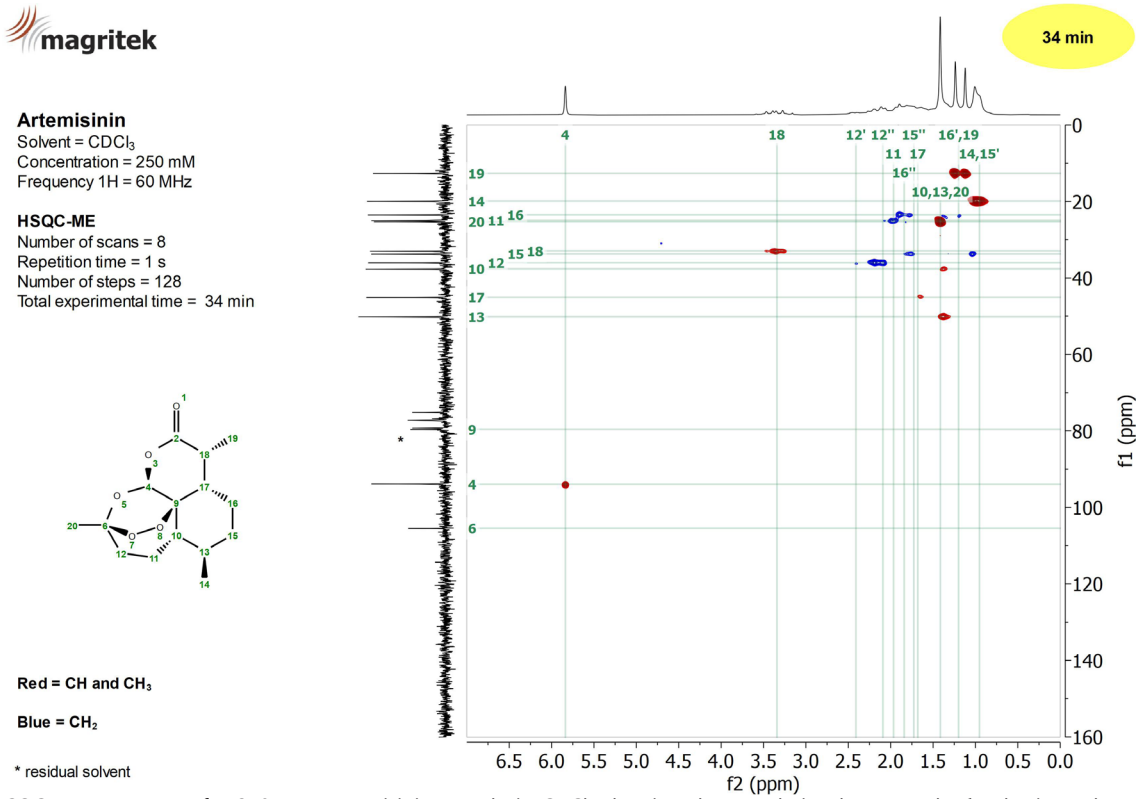

Figure 4: HSQC-ME spectrum of a 250 mM Artemisinin sample in $CDCl_3$ showing the correlation between the ^{1}H (horizontal) and ^{13}C (vertical) signals.

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 Artemisinin sample measured in 68 minutes on our Spinsolve 60 MHz. As an example, the long-range correlation of protons 19 with carbons 2, 17 and 18 are marked. The experiment shows the correlation with quaternary carbons, too.

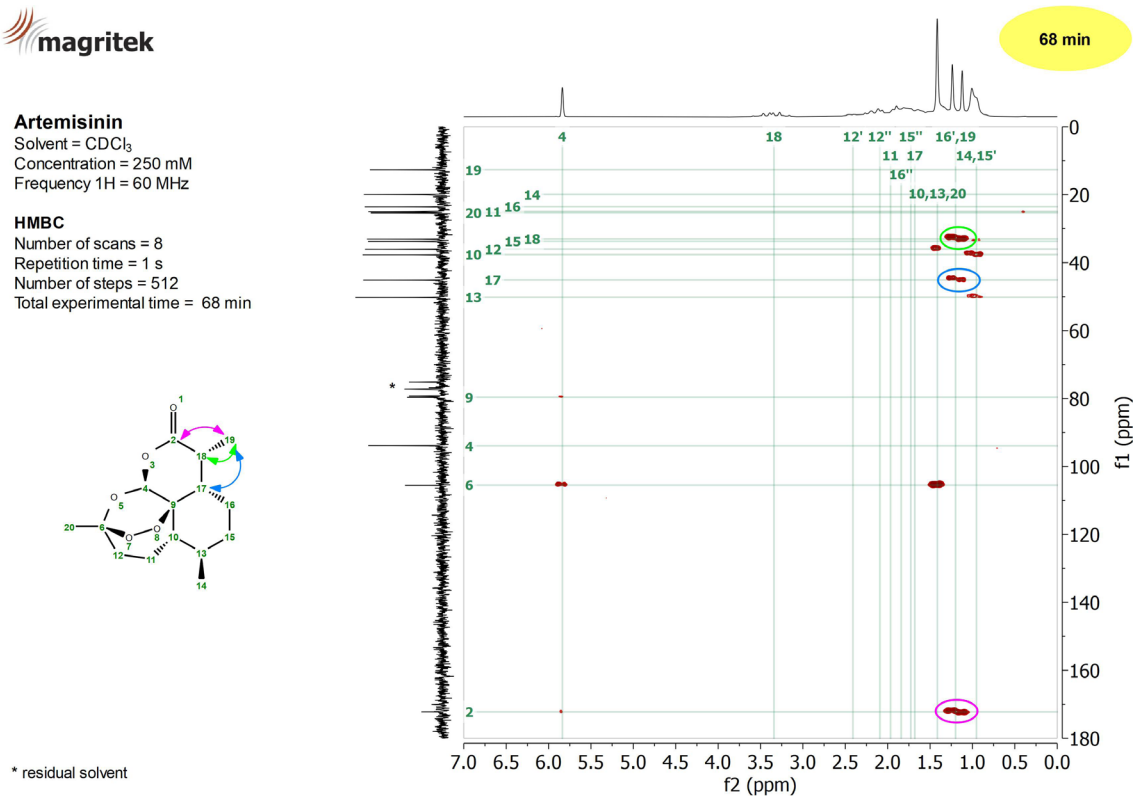

Figure 5: HMBC spectrum of a 250 mM Artemisinin sample in $CDCl_3$ showing the long-range couplings between ^{1}H and ^{13}C nuclei.