Artemisinin

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**

![1D Proton spectrum](image)

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.

![1D Carbon spectrum](image)

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.
The 2D COSY experiment allows one to identify coupled $^1\text{H}$ 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: $^1\text{H}$ 2D COSY experiment of a 250 mM Artemisinin sample in CDCl$_3$ acquired in 17 minutes on a Spinsolve 60 MHz system.

The HSQC is a powerful sequence widely used to correlate $^1\text{H}$ with the one-bond coupled $^{13}\text{C}$ 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 $^1\text{H}$ (horizontal) and $^{13}\text{C}$ (vertical) signals.
2D HMBC

To obtain long-range \(^1\text{H}-^{13}\text{C}\) 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 \(^1\text{H}\) and \(^{13}\text{C}\) nuclei.