Brucine (2,3-Dimethoxystrychnidin-10-one)

Brucine (2,3-Dimethoxystrychnidin-10-one) is an alkaloid, structurally related to strychnine, but less toxic. Figure 1 shows the ^{1}H NMR spectrum of a 250 mM Brucine sample in $CDCl_3$ measured in a single scan taking 10 seconds to acquire.

1D Proton spectrum

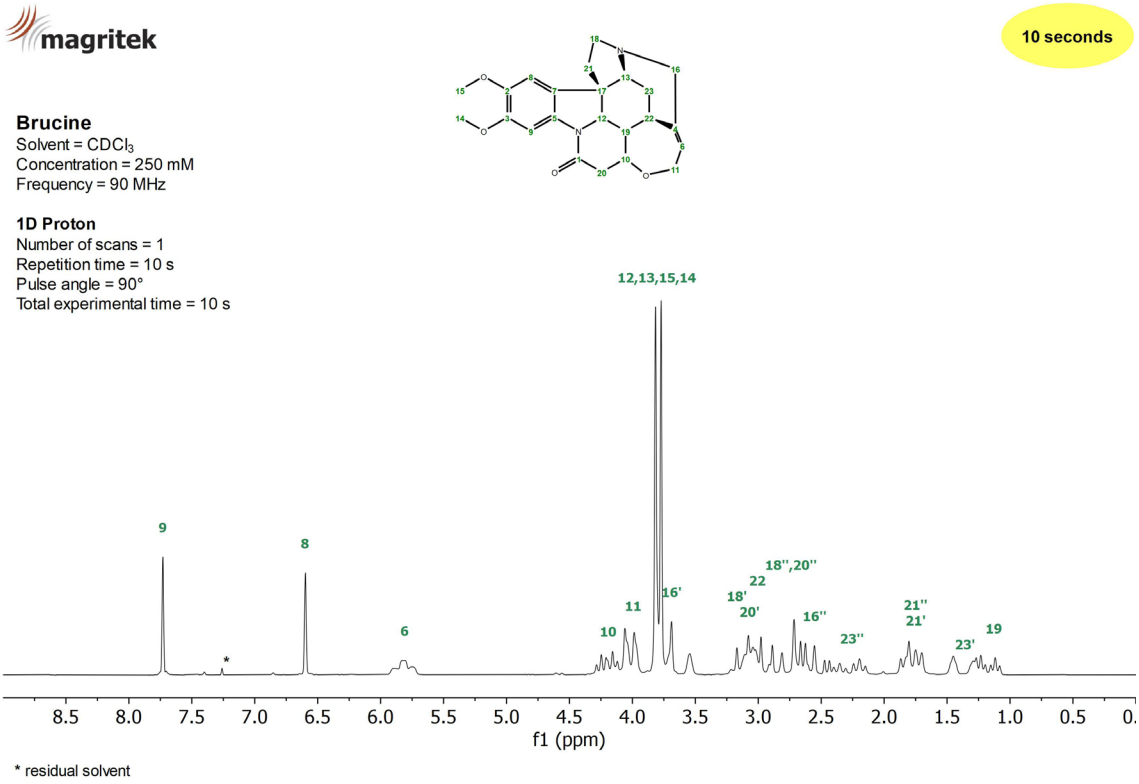


Figure 1: ^{1}H NMR spectrum of a 250 mM Brucine sample in $CDCl_3$ measured on a Spinsolve 90 MHz system in a single scan.

1D Carbon spectrum

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

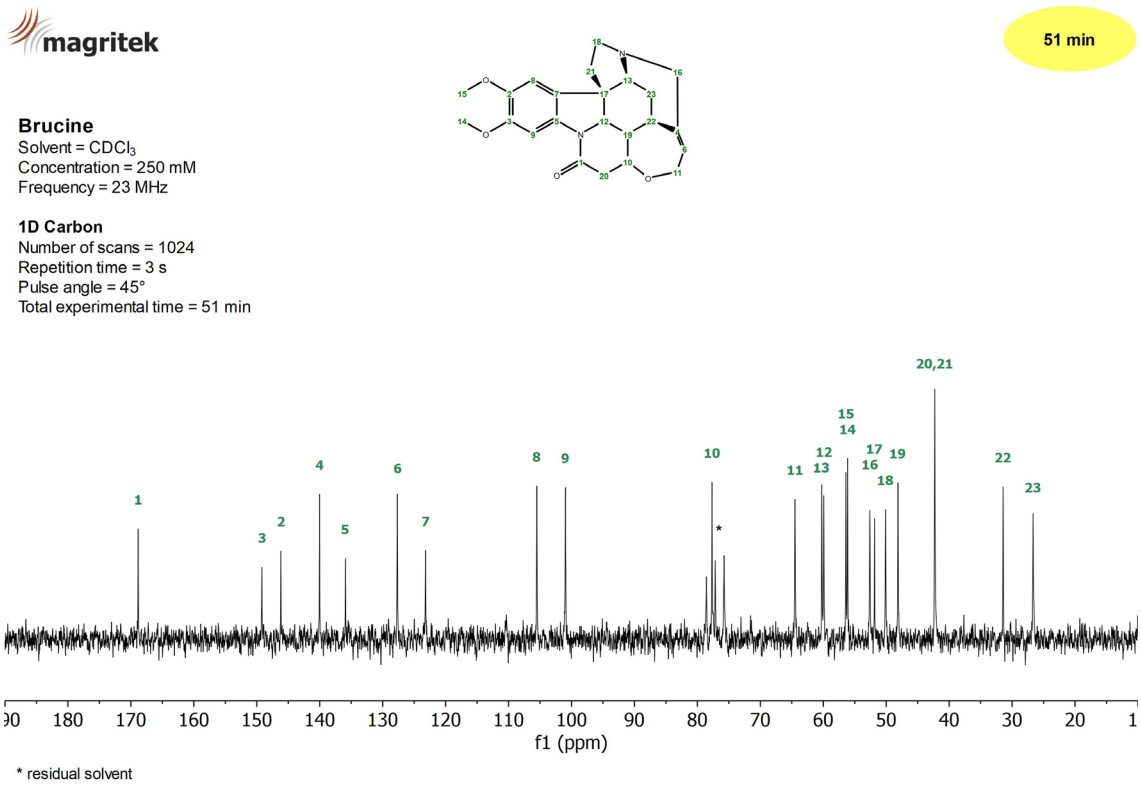
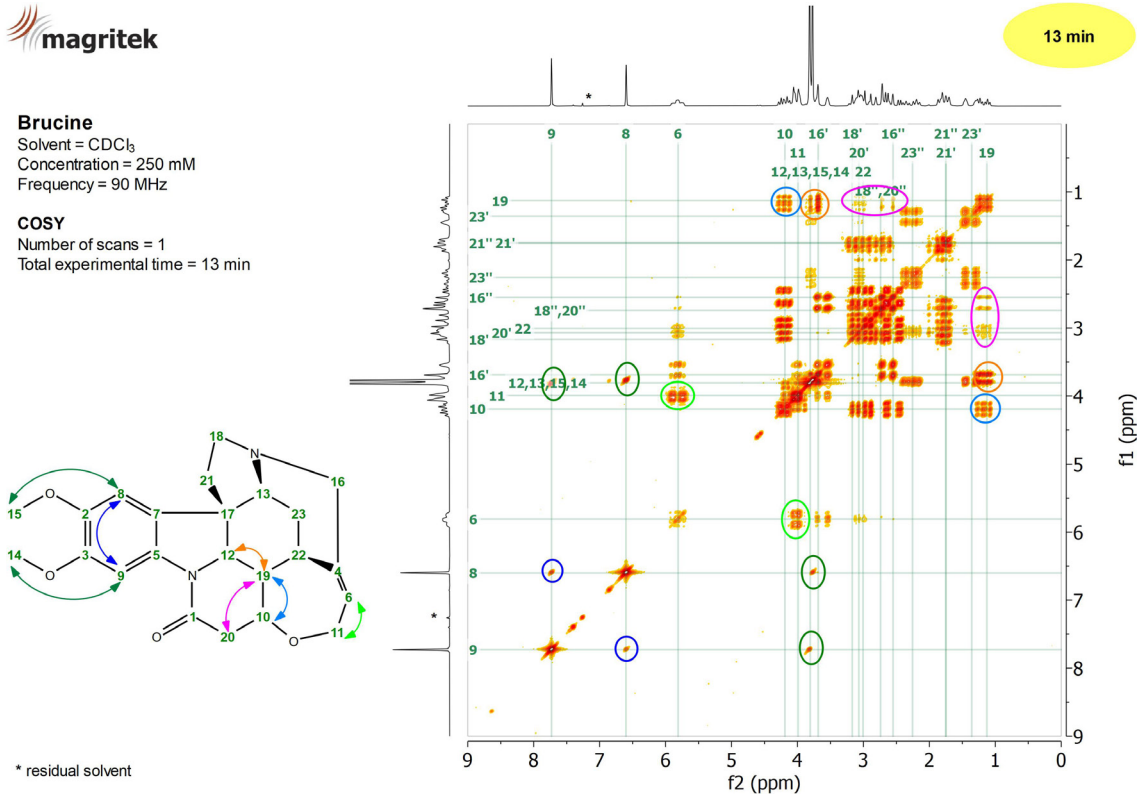


Figure 2: ^{13}C NMR spectrum of a 250 mM Brucine sample in $CDCl_3$ measured on a Spinsolve 90 MHz system in 51 minutes.

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 2 a large number of cross peaks can be nicely observed. For example, the protons at position 6 and 11 (light green) couple with each other. Furthermore, proton 19 couples with proton 10 (light blue), 12 (orange) and 20 (pink). In addition, the couplings between protons 8 and 9 (dark blue) as well as the couplings of protons 8 and 9 with protons 14 and 15 (dark green) can be nicely observed.



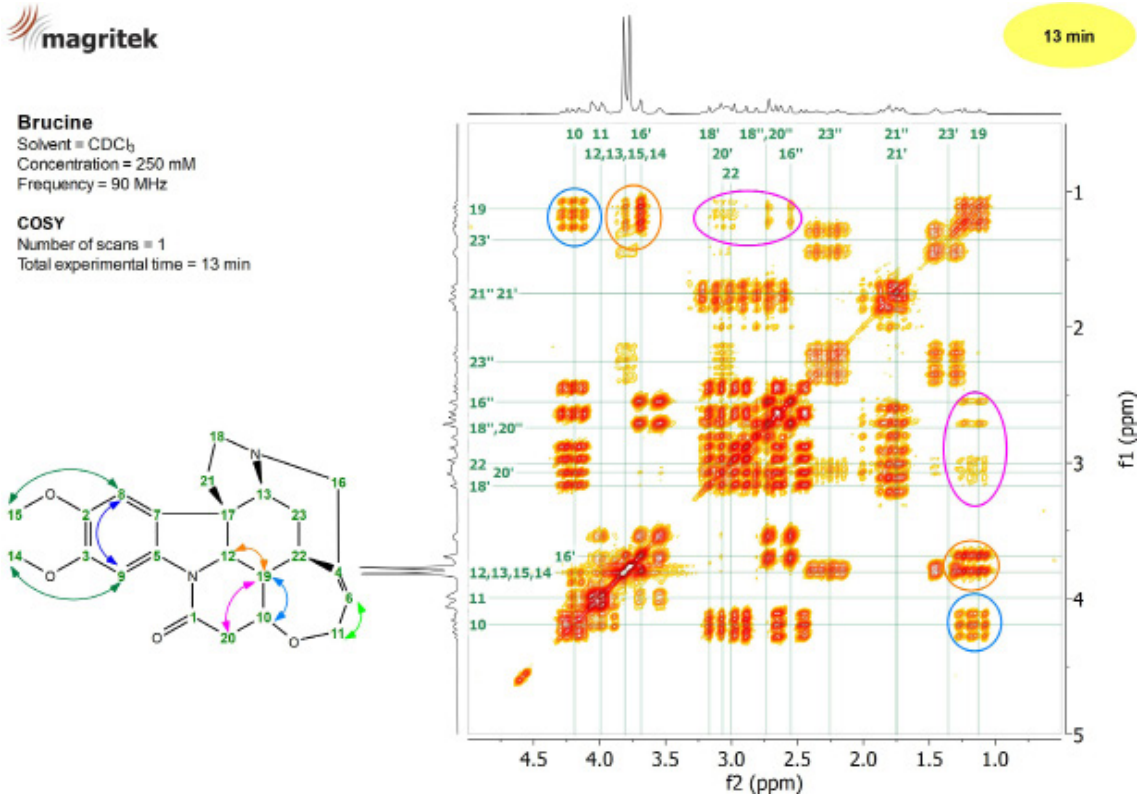


Figure 3: ^{1}H 2D COSY experiment of a 250 mM Brucine sample in $CDCl_3$ acquired in 13 minutes on a Spinsolve 90 MHz system (top); zoom into the aliphatic region (0.5-5.0 ppm) of the ^{1}H 2D COSY spectrum which underlines the superb resolution.

2D JRES spectrum

This 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.

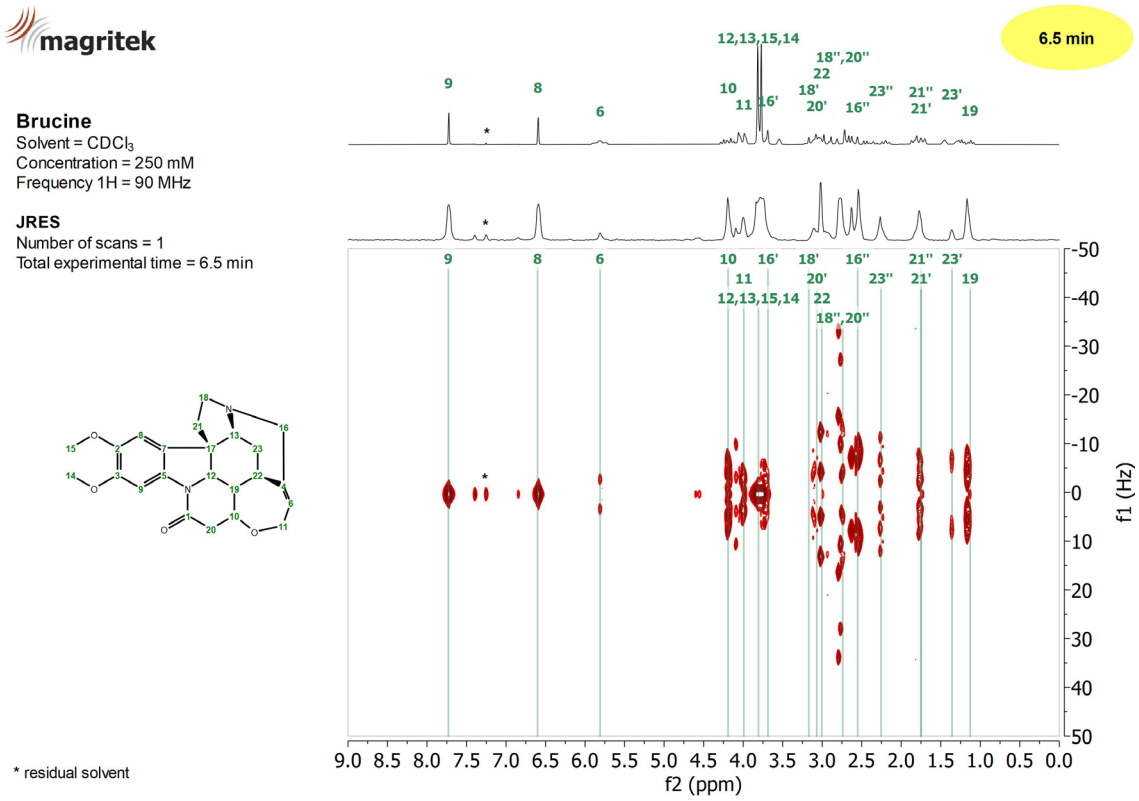


Figure 4: Homonuclear J-resolved (JRES) spectrum of 250 mM Brucine in $CDCl_3$ on a Spinsolve 90 MHz.

2D HSQC-ME

The HSQC is a powerful sequence widely used to correlate the ^{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 between the signals of the CH_2 groups (blue) from the CH and CH_3 groups (red). Figure 5 shows the HSQC-ME spectrum of a 250 mM Brucine sample in $CDCl_3$ acquired in 2 minutes. The measurement time was optimized applying NUS (non uniform sampling).

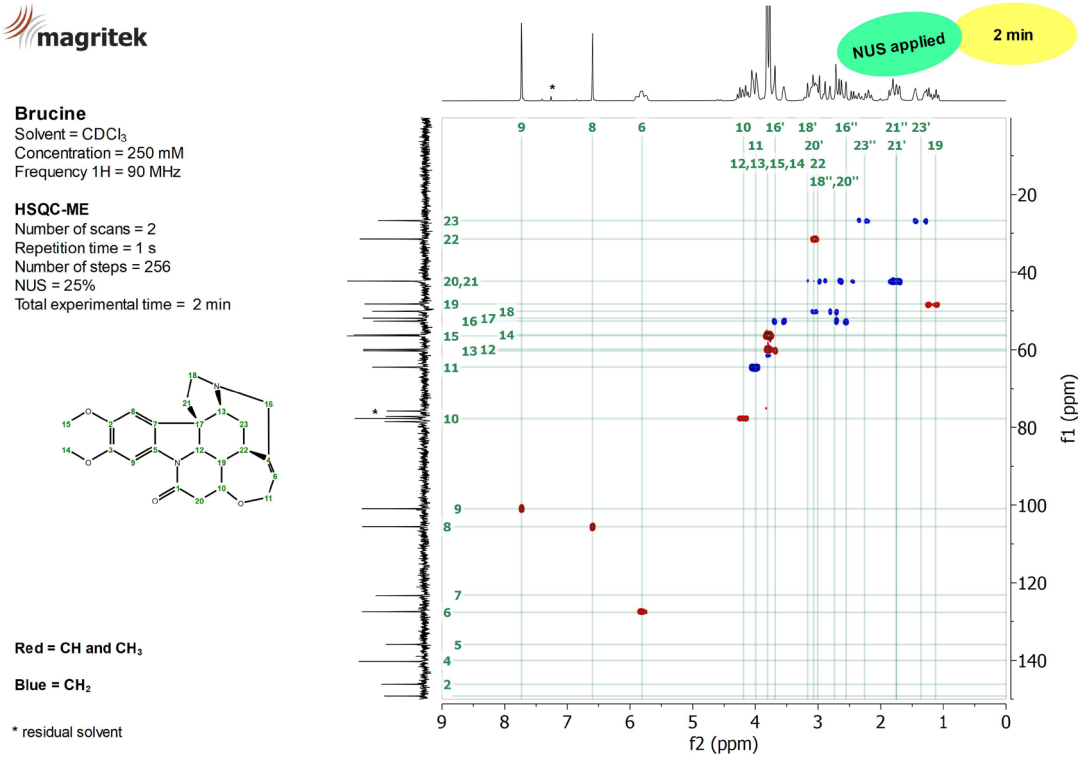


Figure 5: HSQC-ME spectrum of a 250 mM Brucine sample in $CDCl_3$ showing the correlation between the ^{1}H (horizontal) and ^{13}C (vertical) signals.

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 6 shows the long-range correlation of proton 8 with carbons 2, 3, 5, 7, 9 and 17 (the sequence shows the correlation with quaternary carbons, too).

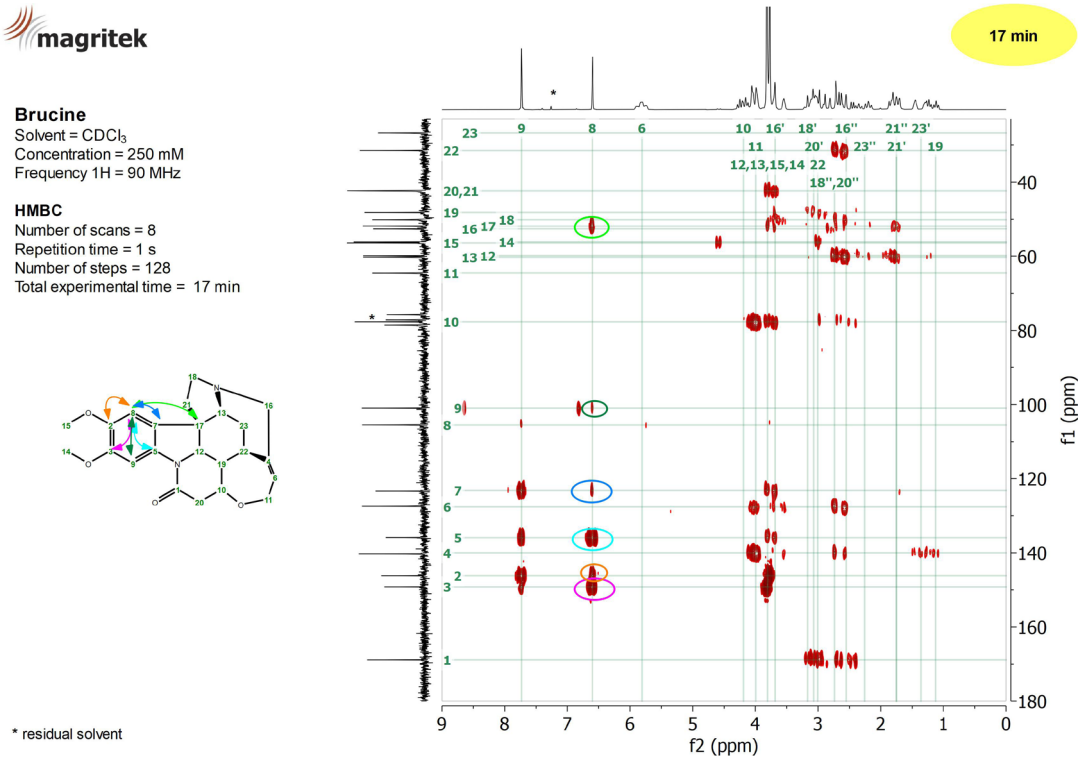


Figure 6: HMBC spectrum of a 250 mM Brucine sample in $CDCl_3$ showing the long-range couplings between ^{1}H and ^{13}C nuclei.