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 100 mM Brucine sample in $CDCl_3$ measured in a single scan taking 15 seconds to acquire.

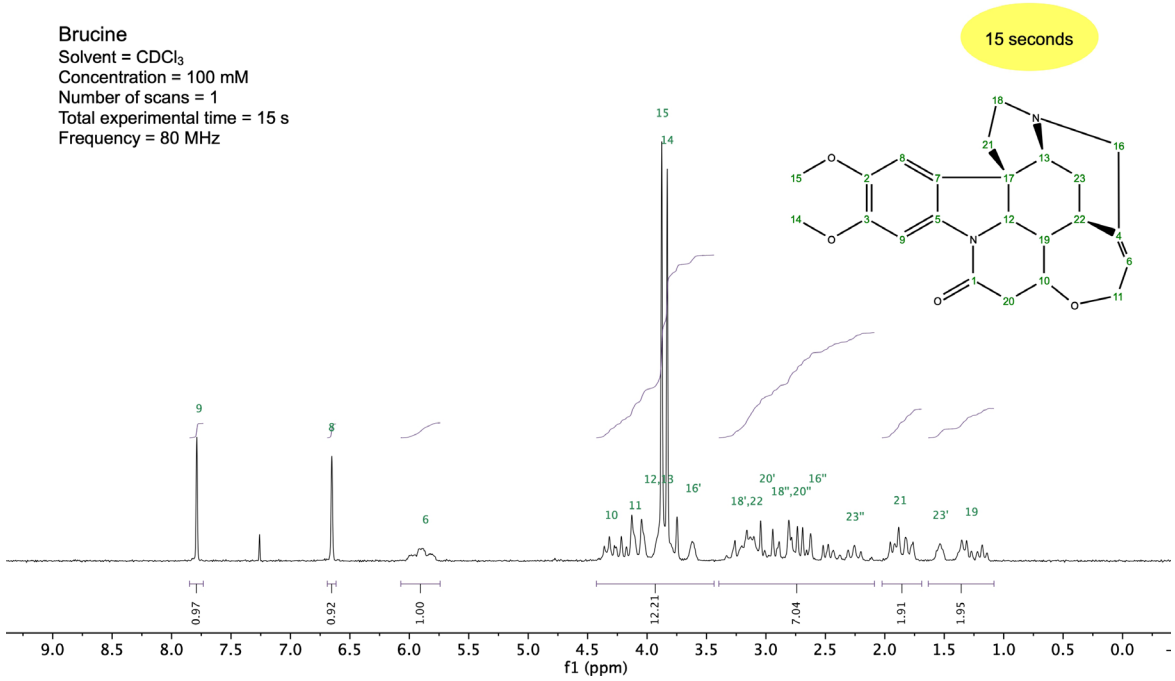

Figure 1: ^{1}H NMR spectrum of a 100 mM Brucine sample in $CDCl_3$ measured on a Spinsolve 80 MHz system in a single scan.

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 2 a large number of cross peaks can be nicely observed. For example, the proton 19 couples to proton 10 (light blue), 12 (orange), and 22 (pink) In addition, the couplings between protons 8 and 9 (dark blue), 8 and 15, 9 and 14 (dark green), 6 and 11 (light green) are marked on the spectrum.

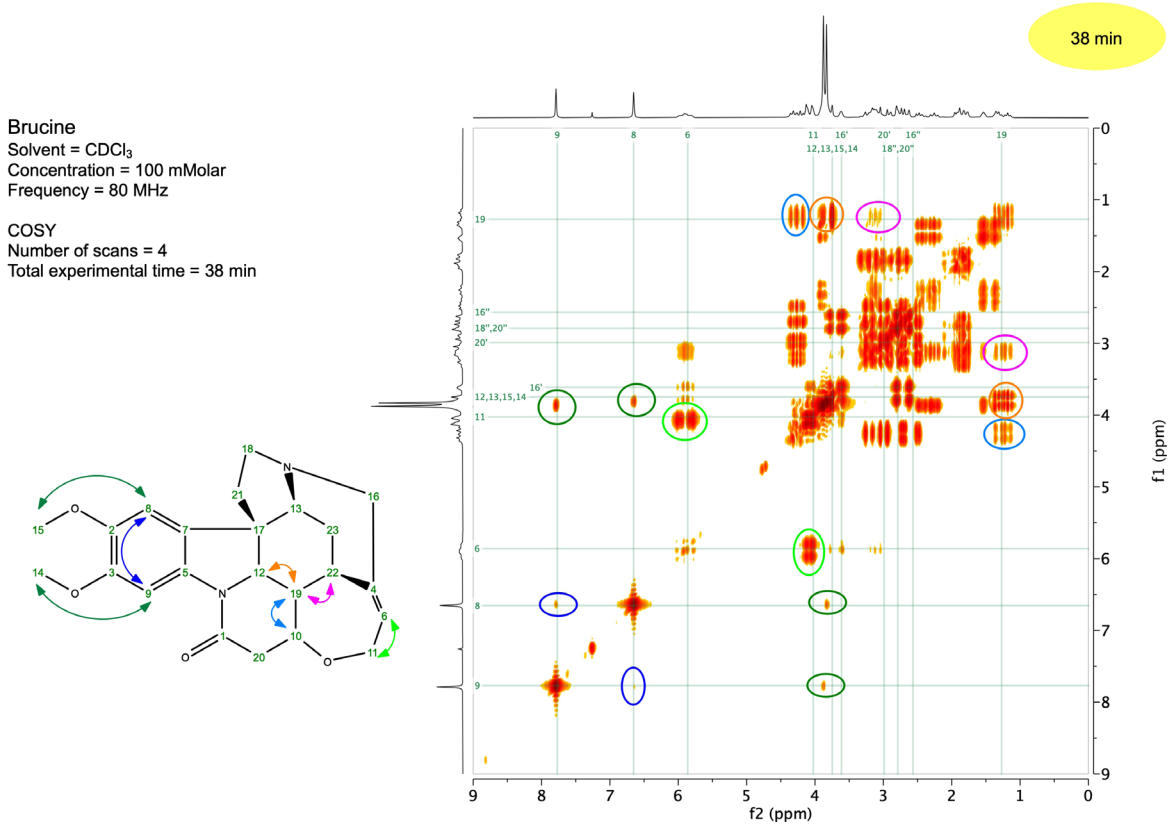

Figure 2: ^{1}H 2D COSY experiment of a 100 mMolar Brucine sample in $CDCl_3$ acquired in 38 minutes on a Spinsolve 80 MHz system.

^{13}C Spectrum

Figure 3 shows the ^{13}C NMR spectrum of 1 M 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.

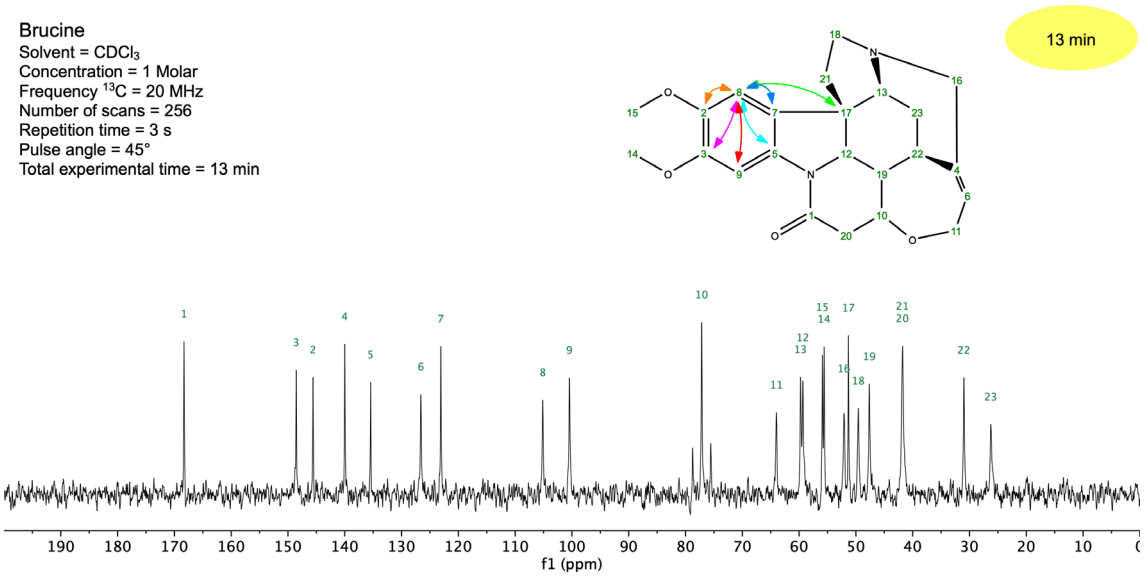

Figure 3: ^{13}C NMR spectrum of a 1 M Brucine sample in $CDCl_3$ measured on a Spinsolve 80 MHz system in 13 minutes. (top).

2D HSQC-ME and 2D HMBC

The HSQC and HMBC are powerful sequences widely used to correlate the one-bond coupled ^{1}H-^{13}C nuclei and long range ^{1}H-^{13}C, respectively. 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 distinguish the signal of the CH_2 groups (blue) from the CH and CH_3 (red). Thanks to the higher sensitivity of these sequences, compared to direct detected ^{13}C experiments, samples with lower concentrations can be measured in relatively short times. Figure 4 shows the HSQC-ME (left) and HMBC (right) spectra of a 300 mM Brucine sample in $CDCl_3$ acquired in 34 minutes per experiment. The HSQC spectrum resolves all coupled ^{13}C and allows one to resolve the ^{1}H signals that overlap in the 1D proton spectrum. On the other hand, the HMBC shows the long-range correlations that are useful to identify and assign the different peaks in the spectrum. As an example, we marked on the HMBC spectrum the cross peaks of proton 8 with carbons 2, 3, 5, 7, 9 and 17 (the sequence shows the correlation with quaternary carbons, too).

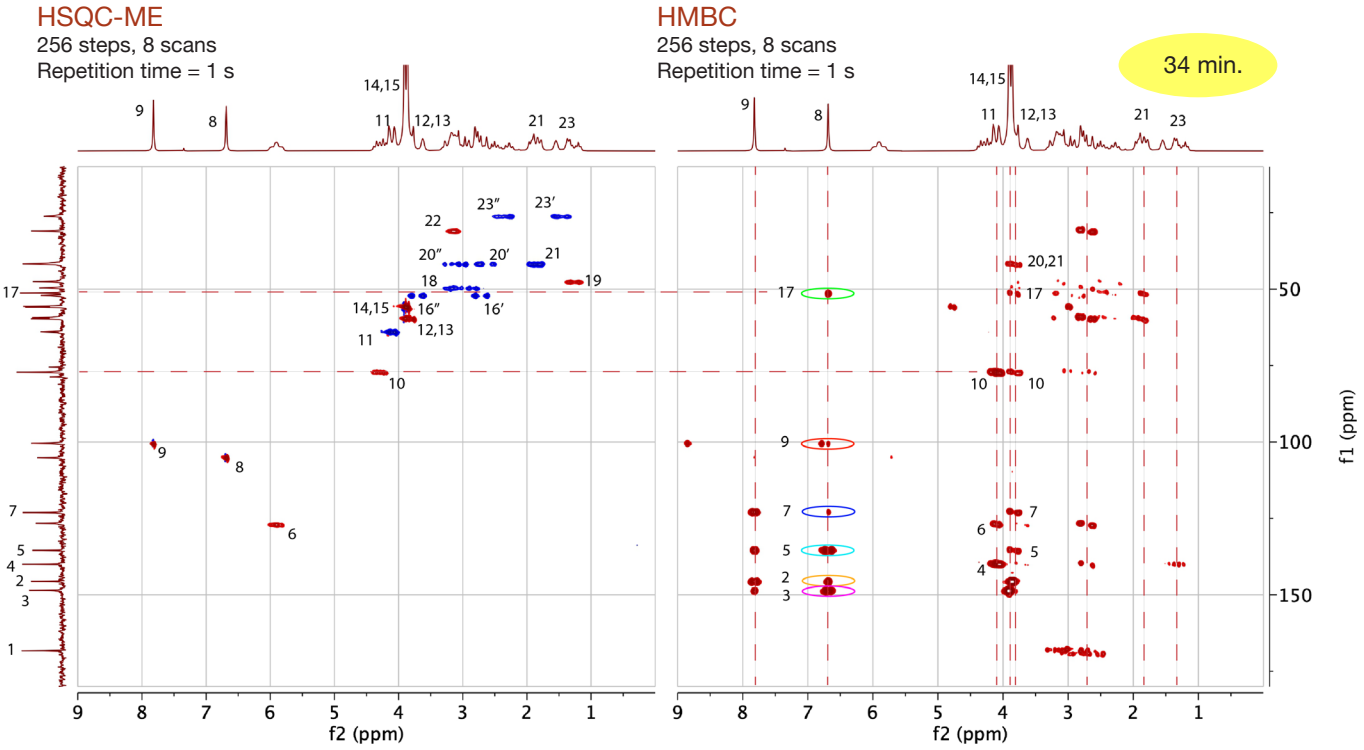

Figure 4: HSQC-ME (left) and HMBC (right) spectra of a 300 mMolar Brucine sample in $CDCl_3$ showing the correlation between the ^{1}H (horizontal) and ^{13}C (vertical) signals.