Gibberellic acid

Gibberellic acid is a plant hormone and the most used substance from the group of Gibberellins. In the industry it is used mainly to stimulate rapid stem and root growth and to speed up the germination. Figure 1 shows the ^{1}H NMR spectrum of a 250 mM Gibberellic acid sample in MeOH-d_4 measured in a single scan taking 10 seconds to acquire.

1D Proton spectrum

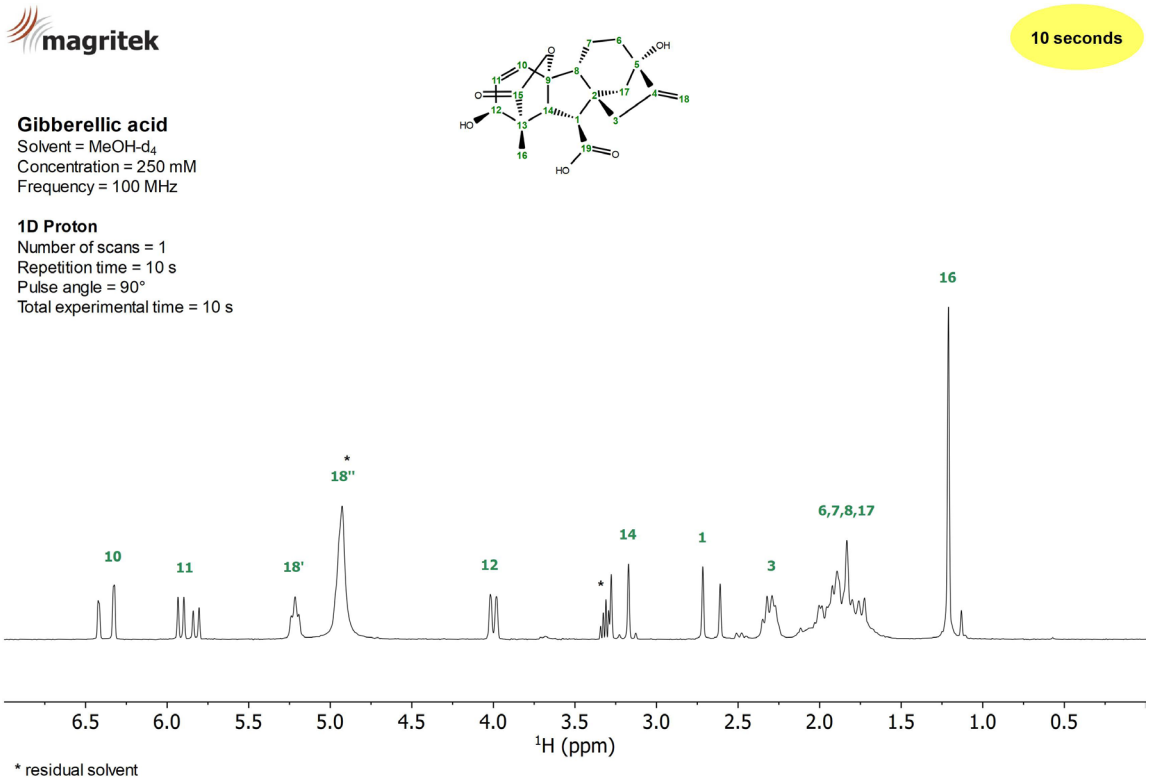

Figure 1: ^{1}H NMR spectrum of a 250 mM Gibberellic acid sample in MeOH-d_4 measured on a Spinsolve 100 MHz system in a single scan.

1D Carbon spectrum

Figure 2 shows the ^{13}C NMR spectrum of 250 mM Gibberellic acid in MeOH-d_4 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.

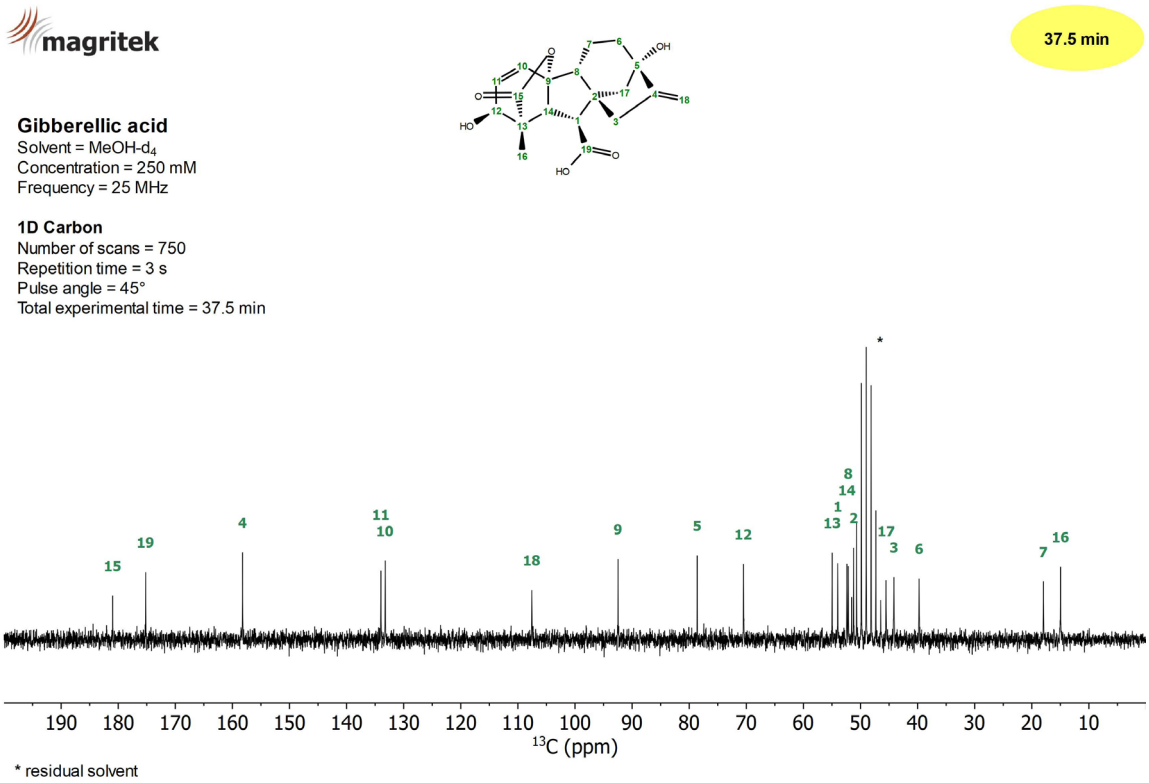

Figure 2: ^{13}C NMR spectrum of a 250 mM Gibberellic acid sample in MeOH-d_4 measured on a Spinsolve 100 MHz system in 37.5 minutes.

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 3 a large number of cross peaks can be nicely observed. For example, the proton at position 11 couples to proton 16 (orange), proton 12 (light green) and proton 10 (dark blue). The proton 16 couples with proton 14 (dark green) and proton 12 (light blue). In addition, the coupling between protons 1 and 14 (pink) can be observed.

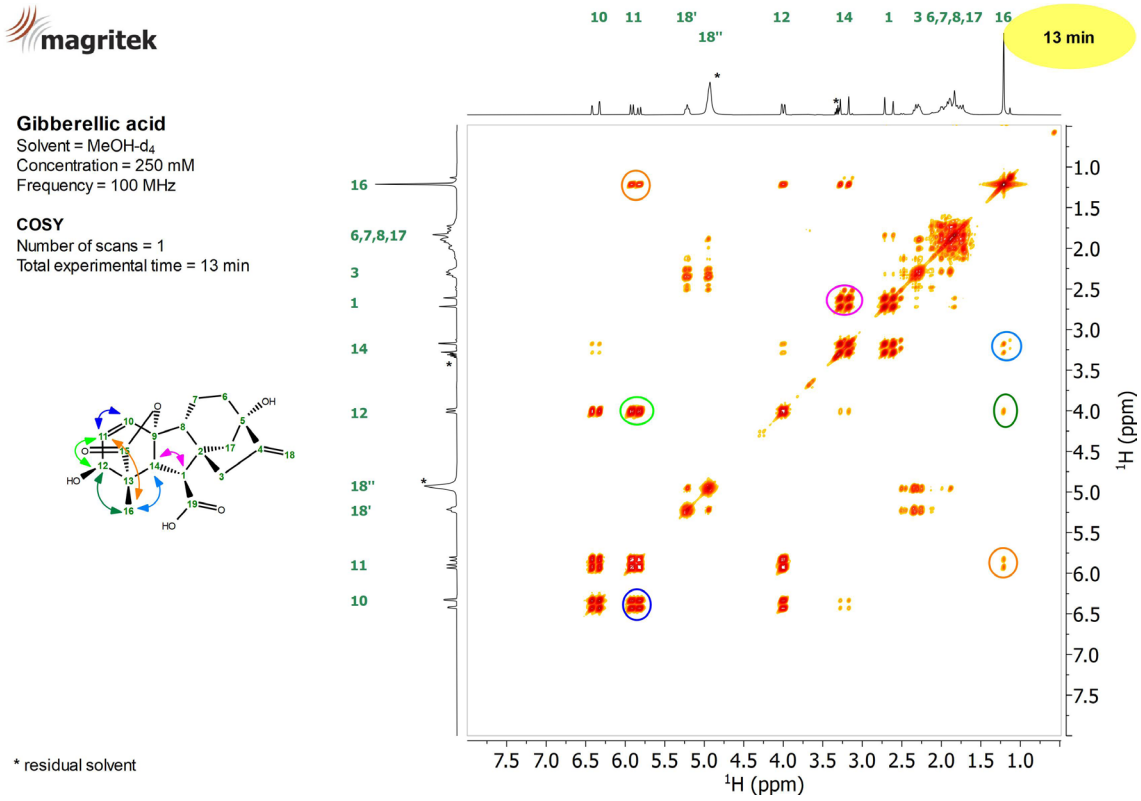

Figure 3: ^{1}H 2D COSY experiment of a 250 mM Gibberellic acid sample in MeOH-d_4 acquired in 13 minutes on a Spinsolve 100 MHz system.

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.

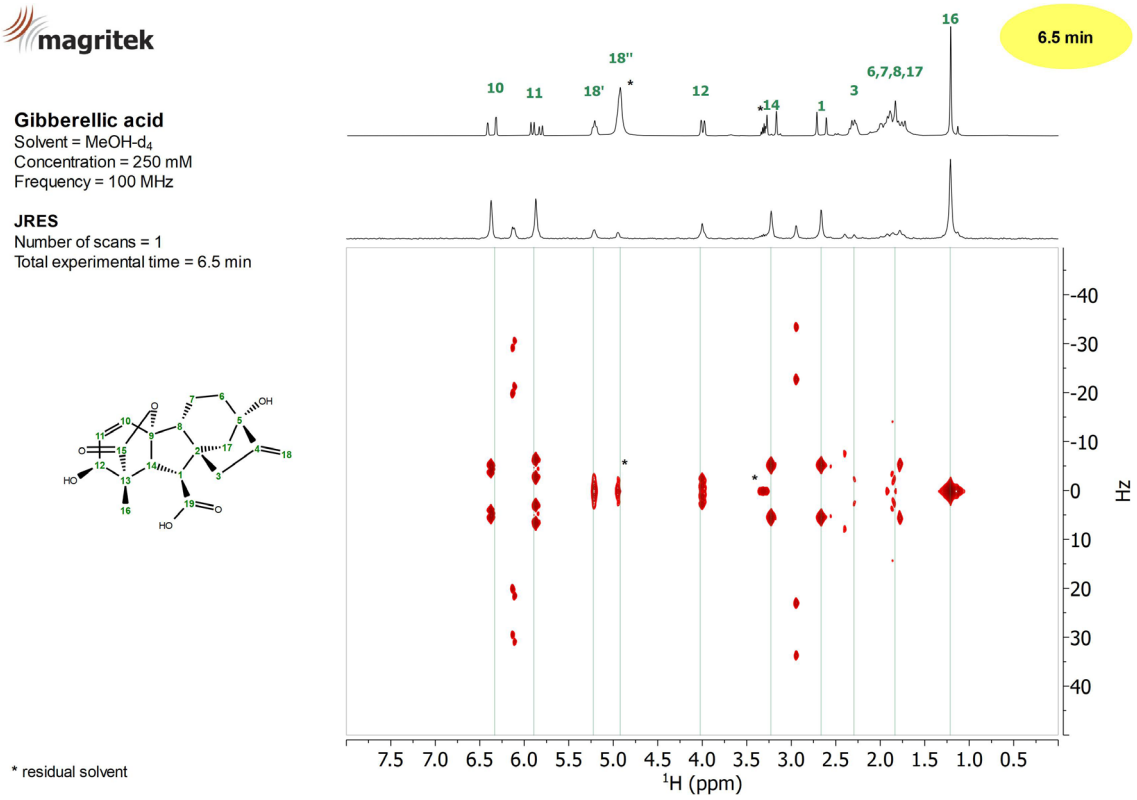

Figure 4: Homonuclear J-resolved (JRES) spectrum of 250 mM Gibberellic acid sample in MeOH-d_4 on a Spinsolve 100 MHz.

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 5 shows the HSQC-ME spectrum of a 250 mM Gibberellic acid sample in MeOH-d_4 acquired in 1 minute. The measurement time was optimized applying NUS (non uniform sampling).

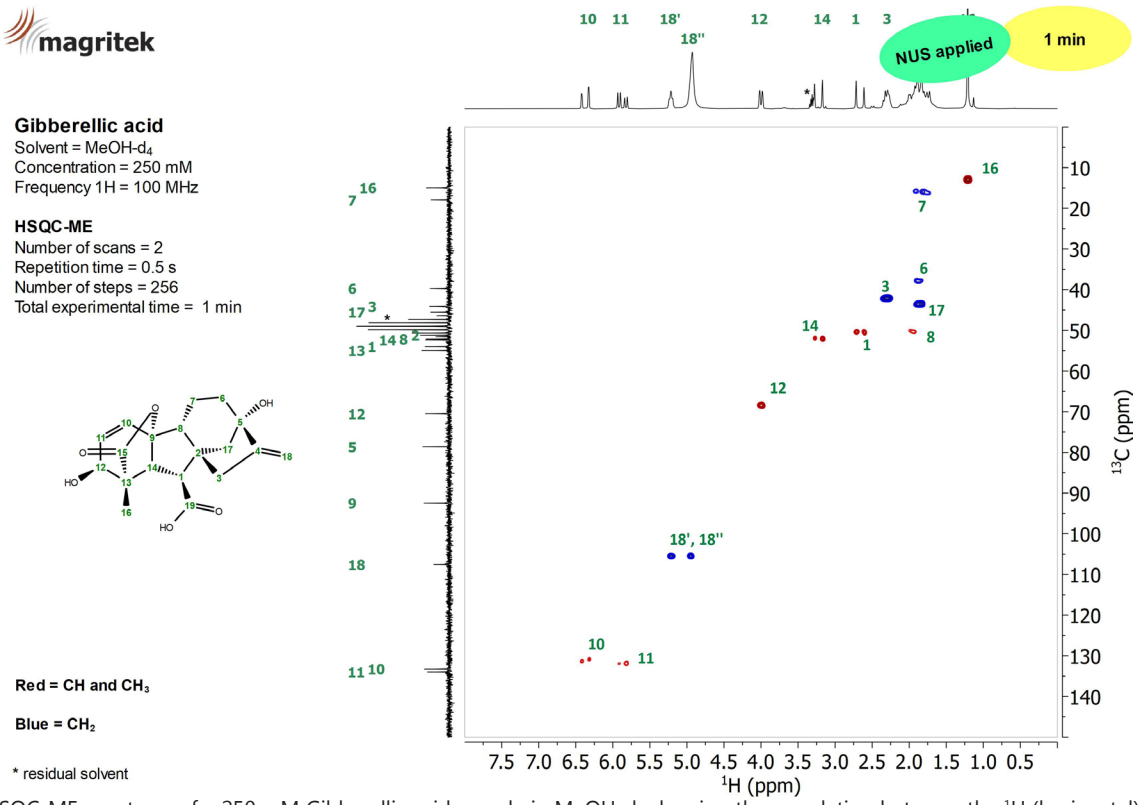

Figure 5: HSQC-ME spectrum of a 250 mM Gibberellic acid sample in MeOH-d_4 showing the correlation between the ^{1}H (horizontal) and ^{13}C (vertical) signals.

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 HMBC spectrum of a 250 mM Gibberellic acid sample measured in 17 minutes on our Spinsolve 100 MHz. As an example, the long-range correlations of proton 11 with carbons 13 (orange), 12 (blue) and 9 (green) are marked with circles. The experiment shows the correlation with quaternary carbons, too.

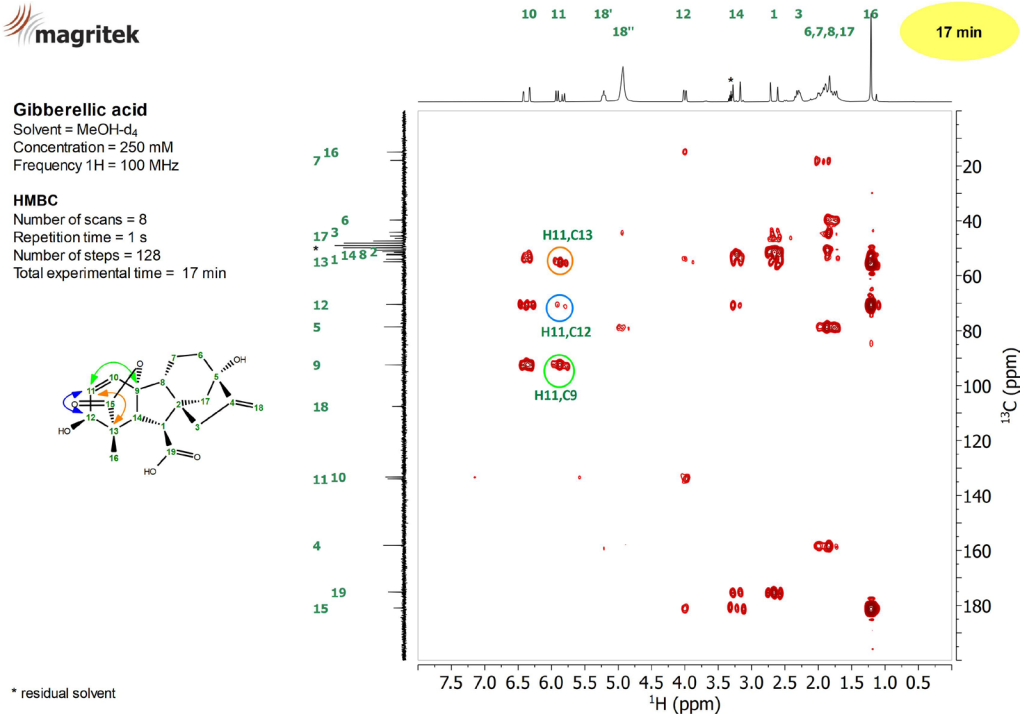

Figure 6: HMBC spectrum of a 250 mM Gibberellic acid sample in MeOH-d_4 showing the long-range couplings between ^{1}H and ^{13}C nuclei.