

## 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  $^1\text{H}$  NMR spectrum of a 250 mM Gibberellic acid sample in  $\text{MeOH-d}_4$  measured in a single scan taking 10 seconds to acquire.

### 1D Proton spectrum

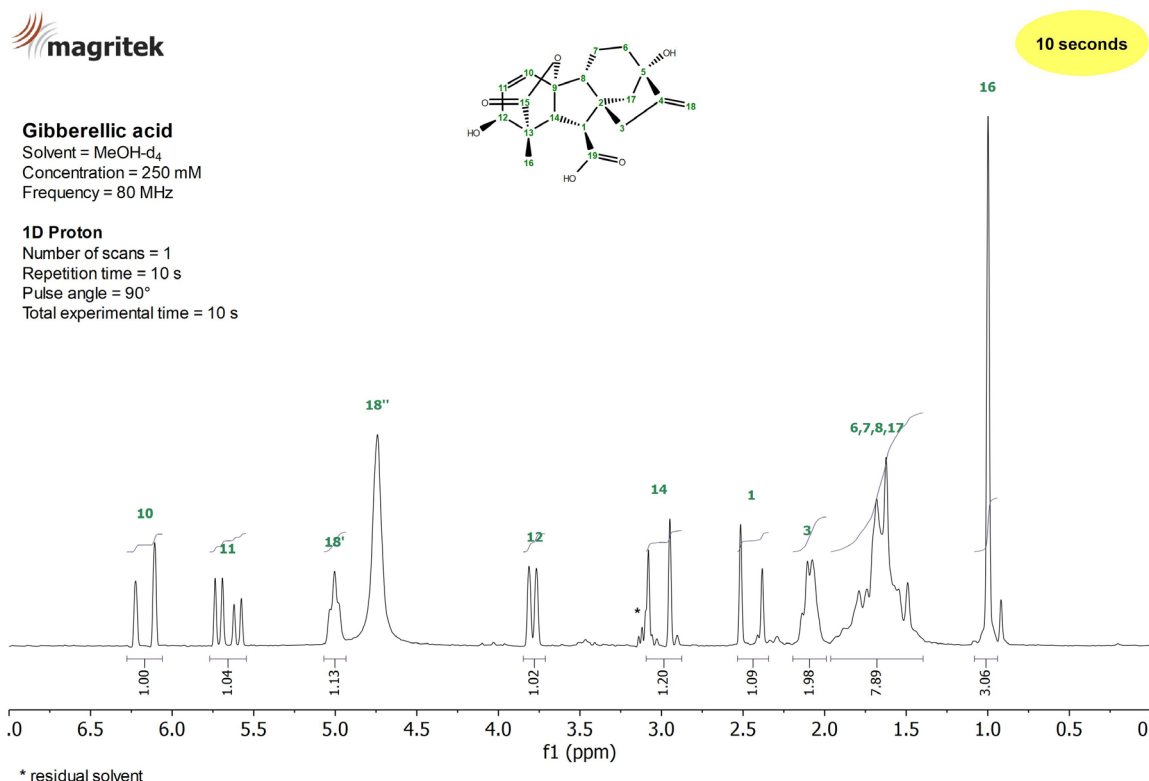


Figure 1:  $^1\text{H}$  NMR spectrum of a 250 mM Gibberellic acid sample in  $\text{MeOH-d}_4$  measured on a Spinsolve 80 MHz system in a single scan.

### 1D Carbon spectrum

Figure 2 shows the  $^{13}\text{C}$  NMR spectrum of 250 mM Gibberellic acid in  $\text{MeOH-d}_4$  acquired using NOE polarization transfer from  $^1\text{H}$  to  $^{13}\text{C}$  and  $^1\text{H}$  decoupling. The 1D Carbon experiment using NOE is sensitive to all  $^{13}\text{C}$  nuclei in the sample. It clearly resolves all the expected resonances.

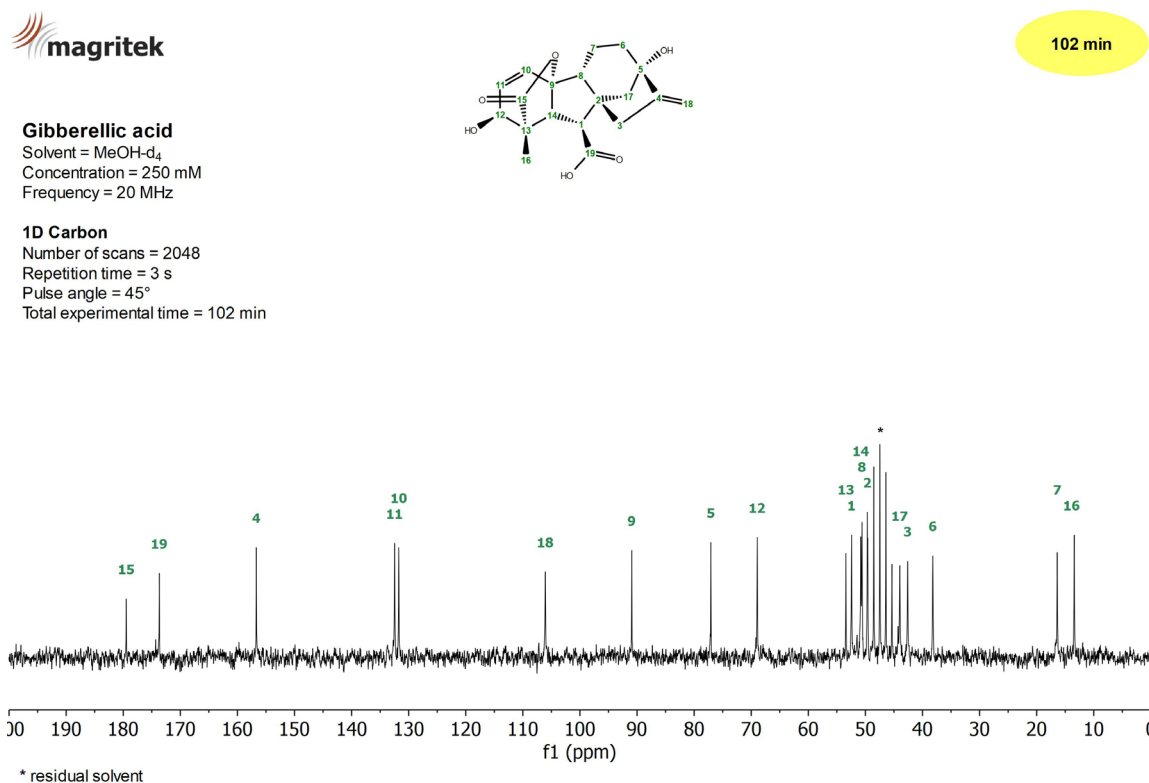


Figure 2:  $^{13}\text{C}$  NMR spectrum of a 250 mM Gibberellic acid sample in  $\text{MeOH-d}_4$  measured on a Spinsolve 80 MHz system in 102 minutes.

## 2D COSY spectrum

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 proton at position 11 couples to protons 16 (orange), proton 12 (light green) and proton 10 (dark blue). The protons 16 couple with proton 14 (light blue) and proton 12 (dark green). In addition, the coupling between protons 1 and 14 (pink) can be observed.

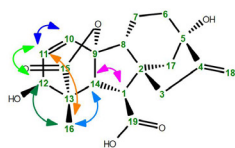


### Gibberellic acid

Solvent =  $\text{MeOH-d}_4$   
Concentration = 250 mM  
Frequency = 80 MHz

### COSY

Number of scans = 1  
Total experimental time = 17 min



\* residual solvent

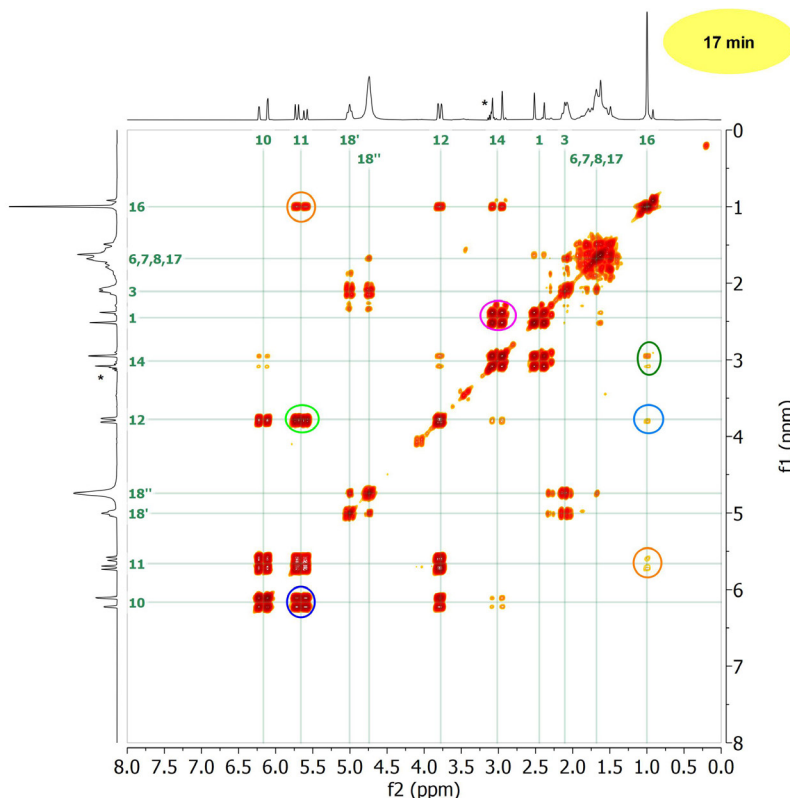


Figure 3:  $^1\text{H}$  2D COSY experiment of a 250 mM Gibberellic acid sample in  $\text{MeOH-d}_4$  acquired in 17 minutes on a Spinsolve 80 MHz system.

## 2D HSQC-ME

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  $\text{CH}_2$  groups (blue) from  $\text{CH}$  and  $\text{CH}_3$  groups (red). Figure 4 shows the HSQC-ME spectrum of a 250 mM Gibberellic acid sample in  $\text{MeOH-d}_4$  acquired in 4 minutes. The measurement time was optimized applying NUS (non uniform sampling).

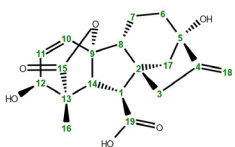


### Gibberellic acid

Solvent =  $\text{MeOH-d}_4$   
Concentration = 250 mM  
Frequency  $^1\text{H}$  = 80 MHz

### HSQC-ME

Number of scans = 2  
Repetition time = 1 s  
Number of steps = 256  
NUS = 50%  
Total experimental time = 4 min



Red =  $\text{CH}$  and  $\text{CH}_3$

Blue =  $\text{CH}_2$

\* residual solvent

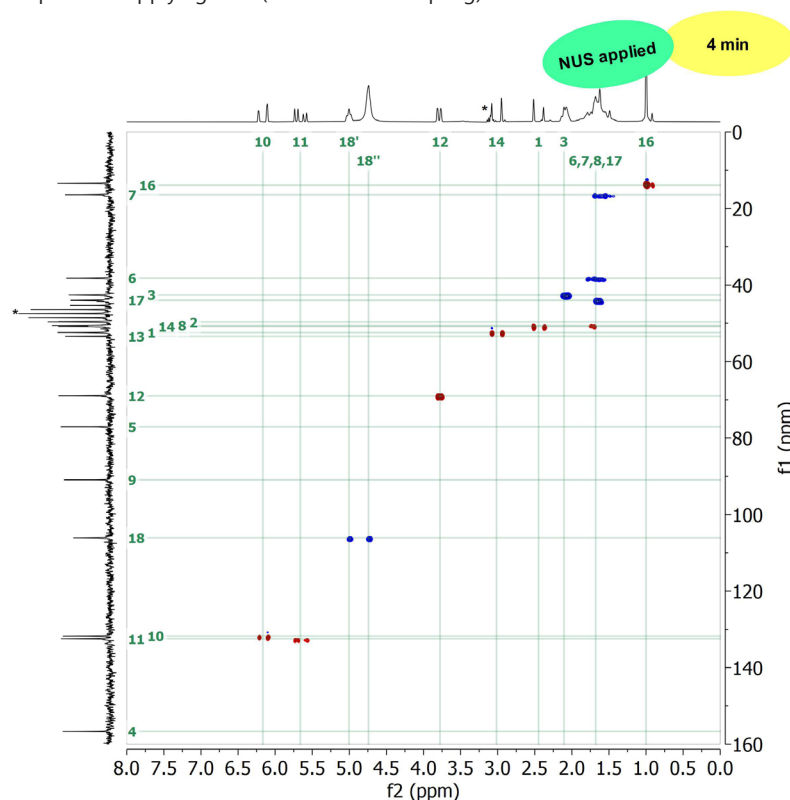


Figure 4: HSQC-ME spectrum of a 250 mM Gibberellic acid sample in  $\text{MeOH-d}_4$  showing the correlation between the  $^1\text{H}$  (horizontal) and  $^{13}\text{C}$  (vertical) signals.

## 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 Gibberellic acid sample measured in 34 minutes on our Spinsolve 80 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.

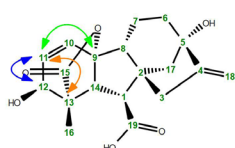


### Gibberellic acid

Solvent = MeOH- $d_4$   
 Concentration = 250 mM  
 Frequency  $^1\text{H}$  = 80 MHz

### HMBC

Number of scans = 8  
 Repetition time = 1 s  
 Number of steps = 256  
 Total experimental time = 34 min



\* residual solvent

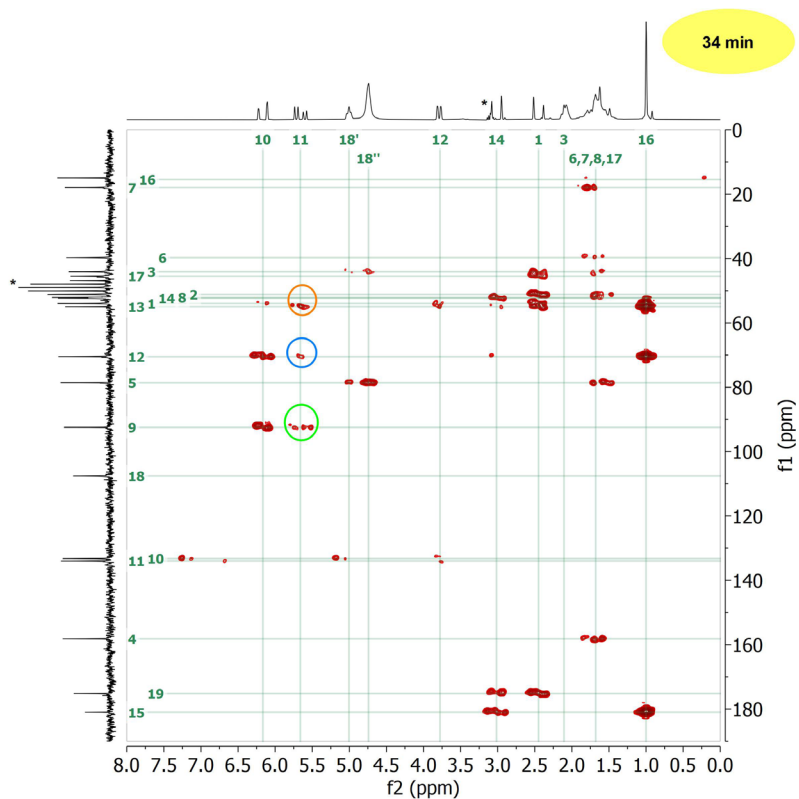


Figure 5: HMBC spectrum of a 250 mM Gibberellic acid sample in MeOH- $d_4$  showing the long-range couplings between  $^1\text{H}$  and  $^{13}\text{C}$  nuclei.