High throughput measurement combining No-D NMR and NUS

Product used : Nuclear Magnetic Resonance (NMR)

No-D NMR is a method to obtain high resolution ^{1}H spectrum without deuterated solvents. It suggests that any reaction mixture or reagent solution are directly available for No-D NMR measurement. Although a huge proton signal of non-deuterated solvent is observed, it could be suppressed by using WET sequence.

On the other hand, since No-D NMR doesn't use NMR LOCK, chemical shift gradually changes during long time experiment. As a result, the line width of NMR signals become broad for long time experiment. Therefore long time experiments (such as 2D measurement) would make less quality data in No-D NMR.

In this note, measurement of high resolution 2D NMR spectra in No-D NMR by combining NUS(Non-Uniform Sampling) is introduced.

Our No-D NMR automation detects and suppresses solvent signals automatically, therefore no need for these messy operations manually. These optimization function can be applied not only to 1D NMR but also to 2D NMR. Therefore multiple 2D experiments can be set continuously without selecting solvent signals and setting the solvent's chemical shift manually.

Fig.1 spectra show high resolution NMR spectrum observed by No-D NMR.

Fig.2.3.4 show general 2D NMR spectra using solvent suppression and NUS. Correlation signals could be observed despite of short measurement time.

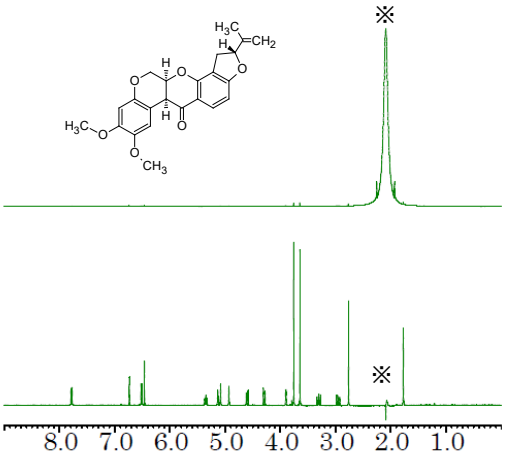

Fig.1: Top : ^{1}H , Bottom : No-D ext time: 1min
(※ solvent signal)

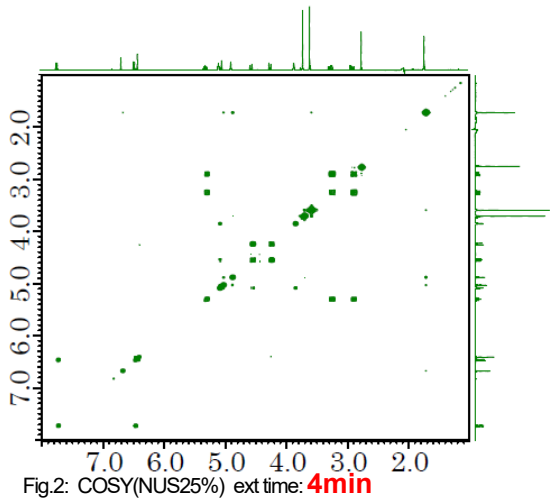

Fig.2: COSY(NUS25%) ext time: **4min**

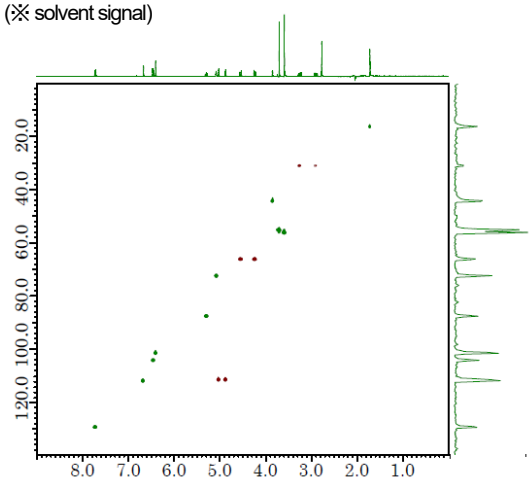

Fig.3: Edited HSQC(NUS25%) ext time: **15min**

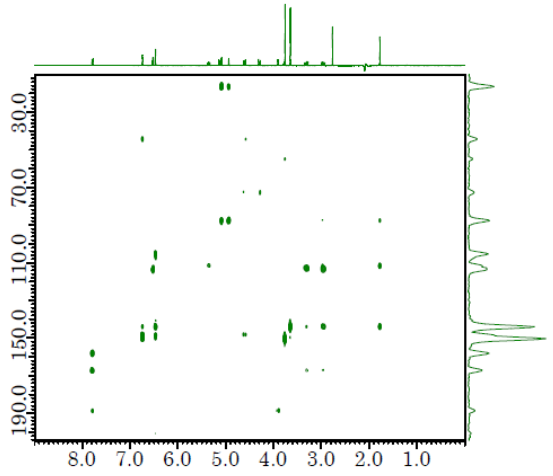

Fig.4: HMBC (NUS25%) spectrum , experiment time: **9min**

Sample : 5mg rotenone/ acetone
Console : JNM-ECZ400S

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