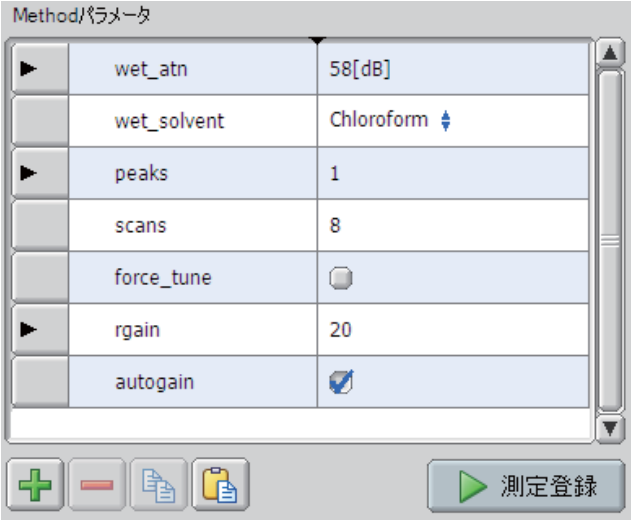
No-D NMR for Delta Version 5

No-D NMR is a method to measure NMR spectra of organic compounds without deuterated solvents. JEOL's latest NMR software, Delta Ver.5, includes automation sequences for No-D NMR, as standard. The sequences can be used more easily than the previous ones, more solvents can be selected, and so more promising.

Advantages of No-D

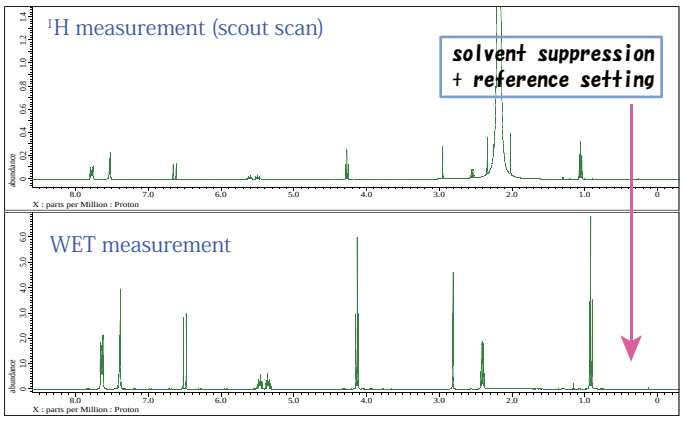
- Time for preparing samples can greatly be reduced, because reaction solutions can be used as they are.
- Unstable samples can be measured, because the process of dissolving samples is omitted.
- The cost for deuterated solvents can be saved.

< Simplified setting parameters and selecting solvents >



When an automation sequence is selected, only the parameters often changed are displayed as method parameters, providing efficient setting.
A measuremtent can immediately be started, when
・wet_solvent: name of solvent
・peaks: number of solvent peaks are set. As standard, 22 normal solvents can be selected, and more solvents can be added on request.
* The othe parameters are in the sub-directory.

< Automatic detection of solvent peaks and adjustment of reference >



CAHE / Acetone

No-D automation sequence starts with a 1-scan ^{1}H measurement to search a solvent signal (scout scan). Then, WET measurement is performed to suppress the solvent signal and also set reference using the signal. Hence, users can save the step of setting reference.

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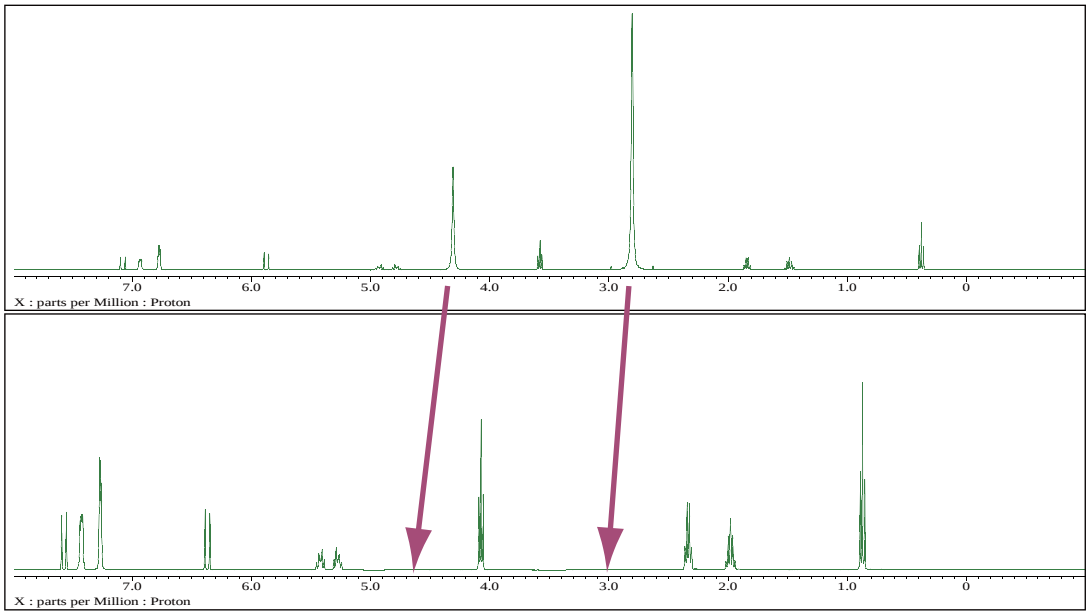
< No-D NMR when a solvent gives more than one peak >

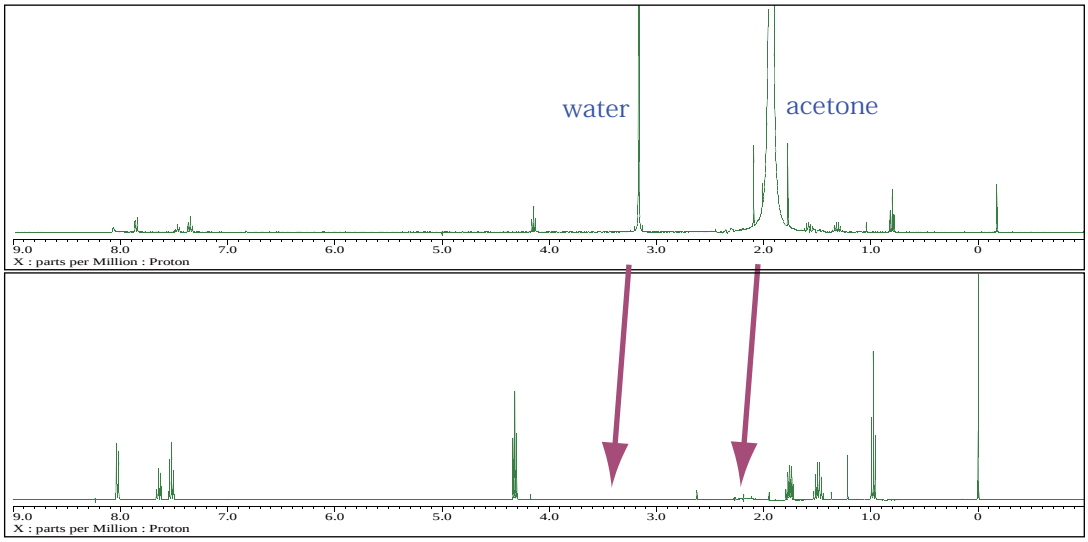
WET sequence has an advantage of suppressing more than one solvent peak at once, and so No-D NMR is applicable to such solvents. In the example of methanol, two peaks are suppressed by setting peaks to be 2.



10% CAHE /Methanol

< No-D NMR when more than one solvent are used >

No-D NMR is applicable to the case when more than one solvents are used. In the example shown below, solvent signals from water and acetone are suppressed.



Butyl benzoate / Water,Acetone

< List of selectable solvents >

acetic acid、acetone、acetonitrile、benzene、chloroform、cyclohexane、DMF、DMSO、ethanol、hexafluoro-2-propanol、isopropanol、methanol、methylene chloride、nitromethane、*o*-dichlorobenzene、*p*-dioxane、pyridine、tetrachloroethane、tetrahydrofuran、toluene、trifluoroacetic acid、trifluoroethanol

* More solvents can be added on request. However, note that adjacent peaks may accidentally suppressed if many solvents are specified.

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