

What is qNMR (quantitative NMR) ?

NMR spectroscopy directly observes atoms (nuclear spins) of molecules, and so it has, in principle, quantitative capability and can be applied to quantification analysis.

Quantitative NMR, or qNMR, is used for determination of concentration and purity of small molecules, for example. This Note introduces **Internal standard method based on ^1H NMR**, where a target compound is not used as a standard material of established purity.

In the method, NMR signal intensities are expressed as Eq. (1), and the purity of the target sample can be calculated using Eq. (2) when the sample is correctly prepared* with an internal standard material of known purity.

$$\text{Eq. (1)} \quad \frac{I_A}{I_B} = \frac{H_A C_A}{H_B C_B} \quad \text{Eq. (2)} \quad P_{\text{sample}} = \frac{I_{\text{sample}} / H_{\text{sample}}}{I_{\text{std}} / H_{\text{std}}} \times \frac{M_{\text{sample}} / W_{\text{sample}}}{M_{\text{std}} / W_{\text{std}}} \times P_{\text{std}}$$

I = Signal intensity (Integral), H = Number of protons in a functional group, C = Concentration, W = Weight, M = Molecular weight, P = Purity (in %)

Fig. 1 shows a ^1H NMR spectrum of diethyl phthalate (DEP) with bistrimethylsilyl benzene (1,4-BTMSB- d_4) as an internal standard. Standard materials should yield an NMR signal not overlapping target signals and have known purity, and 1,4-BTMSB- d_4 with SI-traceability from Wako Pure Chemical Industries, Ltd. is chosen.

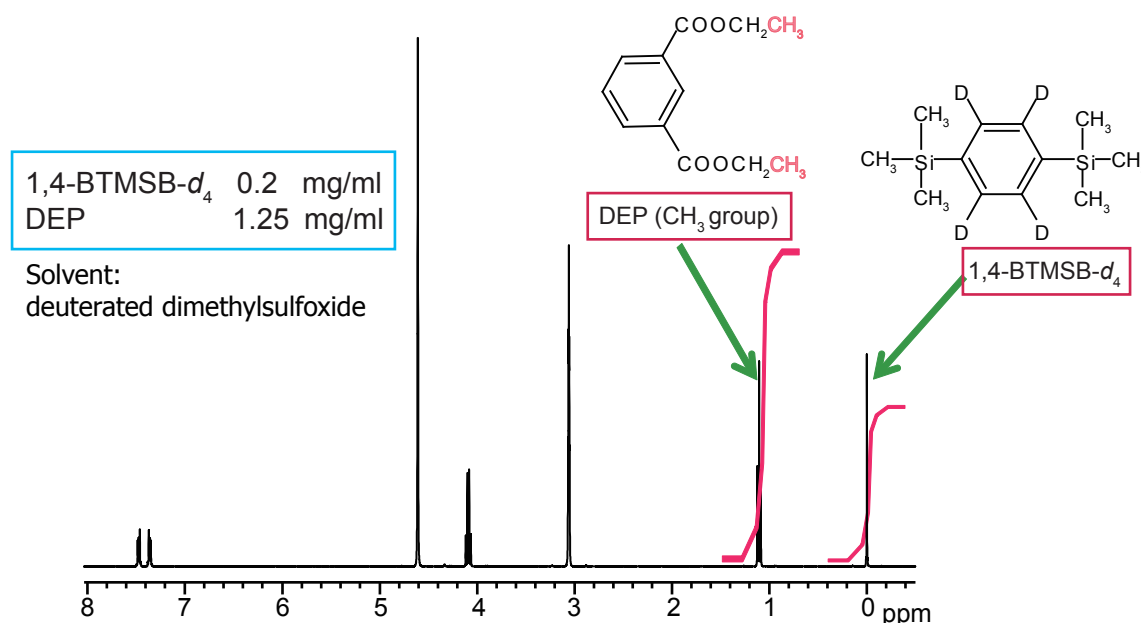


Fig. 1 ^1H NMR spectrum of DEP and 1,4-BTMSB- d_4 (Spectrometer: JNM-ECS400)

* Weighing is necessary for strict sample preparation.