FUJIFILM
Value from Innovation

Wako

Standard for Quantitative NMR

Quantitative NMR (qNMR)

NMR (Nuclear Magnetic Resonance) has been broadly used as a standard analysis method for structural determination of an organic compound. In NMR analysis, the ratio of the number of atomic nuclei in a compound corresponds to the ratio of the areas of the peaks in the spectrum. Therefore, the purity of the compound can be determined by performing a quantitative analysis.

In a purity determination using 1 H NMR, a sample and a standard (an internal standard) having a known purity are mixed together and dissolved in a deuterated solvent. A quantitative value of the sample's purity can be calculated from the relationship among the areas of the spectral peaks originated from the sample and the standard, the numberof protons, the prepared masses, and the molecular weights of the sample and the standard using Formula 1.

【Formula 1】

$$P_{sample} = \frac{S_{sample}}{S_{std}} \times \frac{N_{std}}{N_{sample}} \times \frac{m_{std}}{m_{sample}} \times \frac{M_{sample}}{M_{std}} \times P_{std}$$

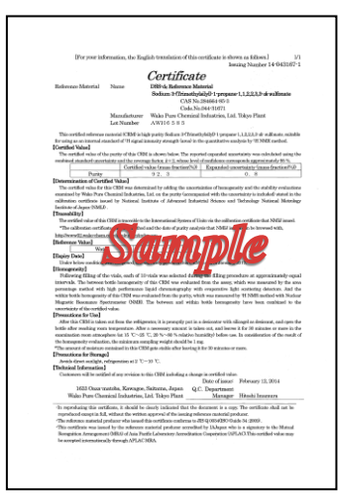
S = Integrated area of the peak
N = Number of protons
(Number of hydrogen atoms in the functional group)
m = Prepared mass
M = Molecular weight, P = Purity

In quantitative analysis using ^{1}H NMR (quantitative NMR), the areas of the peaks of hydrogen atoms observed in the spectrum can be quantitatively compared. Therefore, determination of the purity and quantity of many compounds containing a hydrogen atom is possible with one standard as long as the signals of the sample and the standard do not overlap each other. Highly reliable purity and quantity measurement based on the amount of substance (moles) is possible using a standard certified to be traceable to the International System of Units (SI).

Standard for Quantitative NMR

As a producer of internal standards for quantitative NMR, we acquired accreditation by the ASNITE (Accreditation System of the National Institute of Technology and Evaluation) accreditation program operated by the National Institute of Technology and Evaluation (NITE / IA Japan), and provide the standards as certified reference materials (TraceSure®).The certification gives an uncertainty value as proof of reliability and is attached to every ASNITE accredited and certified reference standard. The certified value described in the certification is internationally accepted through a mutual recognition agreement of APLAC (the Asia Pacific Laboratory Accreditation Cooperation).

We determine a characteristic value of the standard by adding uncertainty obtained from our uniformity evaluation, stability evaluation, etc. to the value of purity (including uncertainty) obtained with a measurement method that is traceable to International System of Units (SI) by the National Metrology Institute of Japan (NMIJ), and we provide the internal standard for quantitative NMR as a reference standard with a certification. Therefore, the characteristic value of the reference standard is traceable to SI through the NMIJ analysis value, and the traceability of the measurements can be shown.

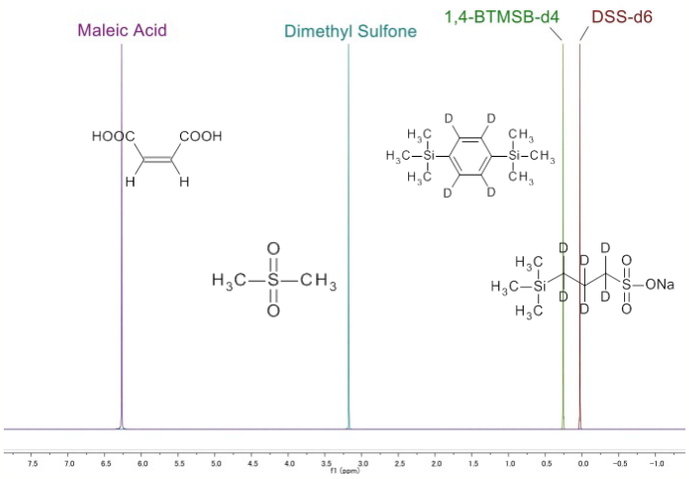

Certificate
Sample

TraceSure Certification

TraceSure® is our series of standards accredited by ASNITE "Reference material producer accreditation" from NITE. ASNITE: Accreditation system of NITE. Accreditation System of National Institute of Technology and Evaluation.

Internal Standard for Quantitative NMR

^{1}H NMR Spectrum (* The chemical shift may vary to some degree depending on conditions.)



Solubility (1000 ppm each when dissolving)

	Maleic Acid	Dimethyl Sulfone	1,4-BTMSB-d_4	DSS-d_6
Acetone-d_6	○	○	○	×
$CDCl_3$	×	○	○	×
D_2O	○	○	×	○
DMSO-d_6	○	○	△	○
CD_3OD	○	○	○	○
CD_2Cl_2	×	○	○	×

■ Standard for Quantitative NMR

Wako Cat. No.	Product Name	Grade	Pkg. Size
024-17031	1,4-BTMSB-d4 Reference Material	TraceSure®	50mg
020-17033			50mg×4
044-31671	DSS-d6 Reference Material	TraceSure®	50mg
040-31673			50mg×4
048-33271	Dimethyl Sulfone Reference Material	TraceSure®	100mg
135-17951	Maleic Acid Reference Material	TraceSure®	100mg
093-06731	4 Internal Standard Set for Quantitative NMR 【Kit Contents】1,4-BTMSB-d4 (50mg×1), DSS-d6 (50mg×1), Dimethyl Sulfone (100mg×1), Maleic Acid (100mg×1)	for qNMR	1set

■ Solvent for NMR [High purity NMR solvent with peaks from impurities suppressed]

Wako Cat. No.	Product Name	Grade	Pkg. Size
031-25531	Chloroform-d, 99.8%(High purity)	for NMR	1mL×5A
040-34571	Dichloromethane-d2, 99.8%(High purity)	for NMR	1mL×5A
044-34471	Deuterium Oxide, 99.8%(High purity)	for NMR	1mL×5A

FUJIFILM Wako Laboratory Chemicals site
https://labchem-wako.fujifilm.com

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