

Reference procedure

¹H-NMR spectroscopy for determination of the quantitative composition of mixtures of structurally known compounds

Proof of competence

ISO/IEC 17025 accreditation

Testing quantities and objects

NMR spectroscopic investigations of organic compounds: Determination of the quantitative composition of simple mixtures of structurally known compounds using $^1\text{H-NMR}$ spectroscopy.

Sample material typically solid (liquid and gaseous/fluid possible) or in solution.

Testing range

Purities expressed as amount of substance (or mass fraction) in relation to total. Amount of substance fractions in the range $1\cdot 10^{-5}$ to 1 (mol/mol) depending on the complexity of the sample.

Expanded measurement uncertainty (k = 2)

Level 1: U = 0.5 to 1.0 % rel., normal operation,

Level 2: U = 0.15 to 0.50 % rel., application measurement, traceability, comparison with high requirements

Level 3: U < 0.15 %, certification of primary standards, interlaboratory comparisons with high requirements

Field of application

Determination of purity or quantification of analytes in organic substances or solutions.

References

F. Malz, H. Jancke, *Journal of Pharmaceutical and Biomedical Analysis* **2005**, *38*, 5, 813-823, https://doi.org/10.1016/j.jpba.2005.01.043.

M. Weber, C. Hellriegel, A. Rueck, J. Wuethrich, P. Jenks, *Journal of Pharmaceutical and Biomedical Analysis* **2014**, *93*, 102-110, https://doi.org/10.1016/j.jpba.2013.09.007.

T. Schönberger et al., Guide to NMR Method Development and Validation – Part I Identification and Quantification *EUROLAB Technical Report* **2014**, *1*, https://eurolab-d.de/dokumente/eurolab/eurolab-technical-reports/.

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