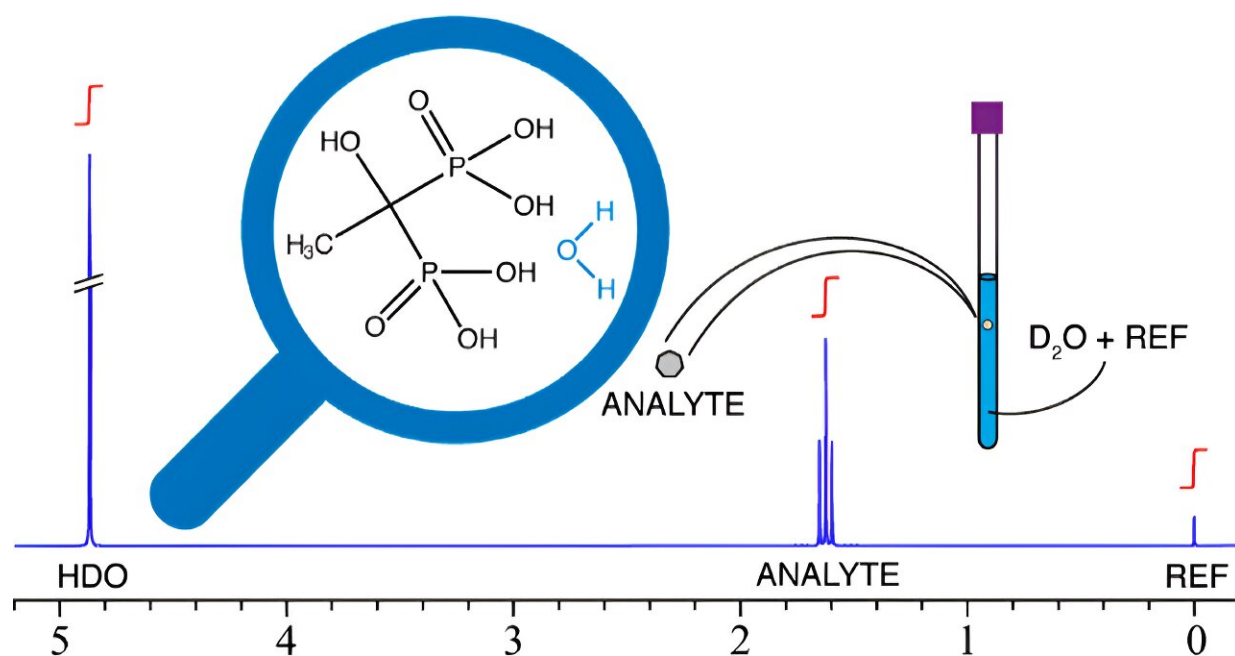


Study offers new method for determining the water content of water-soluble compounds

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Credit: *Analytical Chemistry* (2023). DOI: 10.1021/acs.analchem.3c03689

Researchers at the University of Eastern Finland School of Pharmacy have developed a new method for the accurate determination of the water content of water-soluble compounds. This plays a significant role in, for example, drug dosage. The method utilizes solution-state nuclear magnetic resonance spectroscopy, that is, NMR spectroscopy. The study was [published](#) in *Analytical Chemistry*.

In [pharmaceutical research](#) and development, it is very important to know the exact structure and [water content](#) of the compound being studied, as they affect both the physicochemical and pharmaceutical properties of the compound. Additionally, the water content affects the total molecular weight of the compound that is needed for the calculation of the correct drug dosage.

There are several methods for determining the water content of chemical compounds, of which titration and thermogravimetry (TGA) are the most common ones. However, most methods require accurate weighing, destroy the sample, require special expertise or are time-consuming.

The NMR method developed in the study is simple and accurate and works very well for determining the water content of water-soluble compounds, as the NMR results were comparable with the water contents obtained by TGA and X-ray crystallography determinations.

"The research also revealed that the previously determined water content may change during storage. For example, the commercial sodium salt of citric acid had changed from a form containing 5.5 crystal water molecules to one containing 2 crystal water molecules," Senior Researcher Tuulia Tykkynen and Senior Researcher Petri Turhanen of the University of Eastern Finland point out.

The advantages of the NMR method are easy sample handling (no accurate weighing required), speed (the measurement of one sample and the calculation of the result takes about 15–20 minutes) and the possibility of recovering the investigated compound after the measurement, as the method does not destroy the sample.

The method is also sufficiently precise and repeatable. An NMR spectrometer is a very expensive investment, but it can be stated that the equipment in question is almost always found in laboratories where new

compounds and pharmaceuticals are synthesized, as it is an essential tool for structure determinations.

More information: Tuulia Tynkkynen et al, Simple and User-Friendly Methodology for Crystal Water Determination by Quantitative Proton NMR Spectroscopy in Deuterium Oxide, *Analytical Chemistry* (2023). DOI: [10.1021/acs.analchem.3c03689](https://doi.org/10.1021/acs.analchem.3c03689)

Provided by University of Eastern Finland

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