Results and Analyses of Analemma Water Studied with Nuclear Magnetic Resonance (NMR) and Fourier Transform Infrared Spectroscopy (FT-IR)

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Summary

Water is one of the most studied and, at the same time, one of the most intriguing substances in nature. Although its chemical formula – H_2O – appears simple, its behavior is determined by a complex and dynamic network of hydrogen bonds between individual molecules. This network influences the physical properties of water, its structure in different environments, the way its molecules interact with one another, and the formation of groups of water molecules – water clusters.

The study presents results obtained by two modern spectroscopic methods — Nuclear Magnetic Resonance (NMR) and Fourier Transform Infrared (FT-IR) Spectroscopy. NMR makes it possible to monitor changes in the chemical shifts, which provide information about the molecular environment and the dynamics of water molecules. FT–IR analysis complements this picture by revealing features of O–H vibrations associated with hydrogen bonds and the possible formation of water clusters.

The aim of the study is to compare the spectral characteristics of Analemma Water with those of a control distilled water sample, to identify possible differences in the organization of the hydrogen-bond network, and to evaluate water clusters.

Experimental conditions:

Control sample: Distilled water not exposed to any external treatment.

Experimental sample:

A sample of distilled water was exposed to the **Analemma Water Inlay** for 10 minutes under identical and controlled experimental conditions.

1. Nuclear Magnetic Resonance (NMR)

The nuclear magnetic resonance (NMR) spectra were measured on a Bruker Avance II+ 600 spectrometer **(**Bruker BioSpin GmbH Rheinstetten, Germany) using a 5 mm direct-detection dual-broadband probe. The experiments were performed at a temperature of 298 K. ^{1}H NMR spectra were acquired with 128 K time-domain points, a spectral width of 9600 Hz, 16 scans, and a relaxation delay of 60 s. The chemical shifts were referenced to the residual dmso-d6 resonance used as an external reference (2.5 ppm). The dmso-d6 was placed in a coaxial capillary in the sample tube and used as a lock signal.

Figure 1 demonstrates NMR results of Analemma water (a) and the Control sample (b) of distilled water

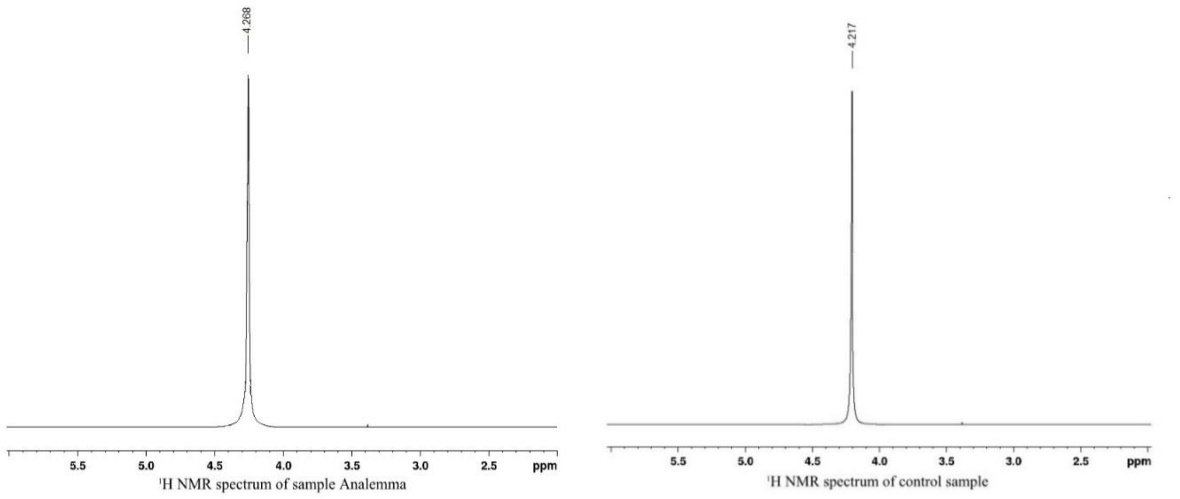

Figure 1. NMR results of Analemma water (a) and Control sample (b) of distilled water

Table 1. Chemical shifts (δ, ppm) and $\Delta\nu_{1/2}$, Hz of a sample of Analemma water and Control sample of distilled water

Sample	**δ, ppm**	**$\Delta\nu_{1/2}$, Hz**	**Comment**
1	4.268	8.37	Sample of Analemma water
2	4.217	6.21	Control sample of distilled water

The difference between the sample and the control sample for the chemical shift is
Δδ, ppm = δ, ppm (Analemma water) – δ, ppm (control)
= 4.268 – 4.217 = 0.051 ppm

The result for Analemma water, compared with the control sample, is reliable.

The obtained results demonstrate measurable differences between the **Analemma Water** sample and the control sample. In the **NMR analysis**, a difference in chemical shift was observed: the Analemma Water sample signal was recorded at **δ = 4.268 ppm**, whereas the control sample was recorded at **δ = 4.217 ppm**. The chemical-shift difference, **Δδ = 0.051 ppm**, indicates a change in the local molecular environment of the water protons, which may be associated with differences in hydrogen-bond organization and proton shielding.

In addition, the difference in the NMR linewidth,

$\Delta\nu_{1/2}$, Hz = $\Delta\nu_{1/2}$, Hz **(Analemma water) –** $\Delta\nu_{1/2}$, Hz **(control) =**

=8.37 – 6.21 = 2.16 Hz

suggests differences in the dynamics of molecular interactions. Since the linewidth is related to relaxation processes, the observed increase may reflect altered proton relaxation behavior, potentially connected with changes in the cooperative hydrogen-bond network and the formation or rearrangement of water molecular clusters. These results suggest that the Analemma Water sample exhibits modified intermolecular organization compared with the control distilled water sample, particularly with respect to hydrogen-bond dynamics and cluster structuring.

2. Modeling of Water Clusters with Fourier Transform Infrared (FT-IR) Spectroscopy

The water samples were analyzed using Fourier-transform infrared (FT-IR) spectrometry. The FT-IR spectra in our study were recorded with a “Thermo Nicolet Avatar 360 FT-IR” spectrometer (Waltham, MA, USA), equipped with a DTGS detector in the region 400–4000 cm^{-1}, accumulating 64 scans at a spectral resolution of 2 cm^{-1}. The experiments with FT-IR were performed at 298 K.

FT–IR records how water absorbs infrared light, which depends on the vibrations of molecular bonds. When these data are combined with molecular modeling, it is possible to propose model-consistent interpretations of cluster-related vibrational features and their dynamics in Analemma Water. This allows assessment of vibrational features that may be consistent with specific hydrogen-bonding environments or hydration motifs.

Figure 2 demonstrates the FT-IR spectrum of Analemma Water

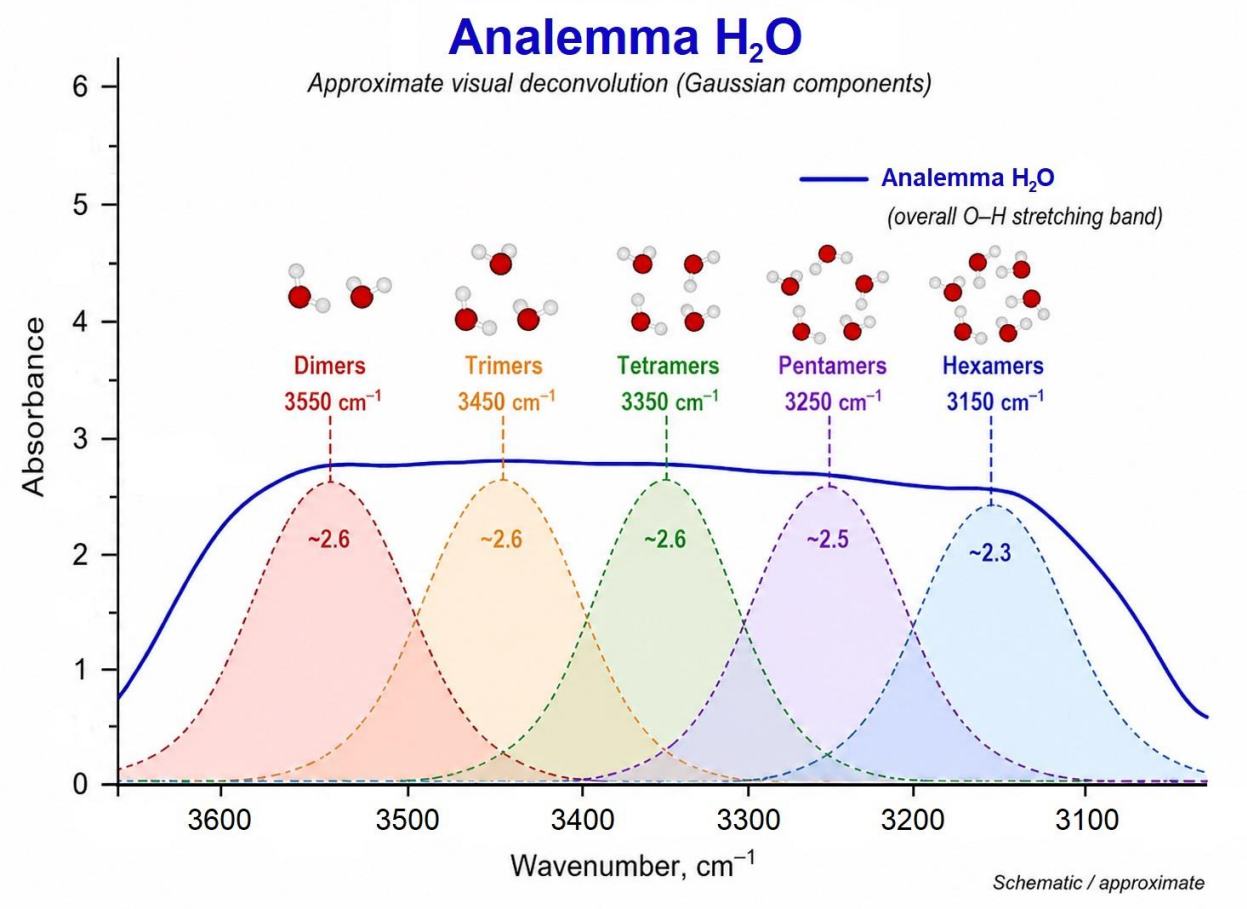

Figure 2. FT-IR spectrum of Analemma Water

The peaks in the infrared (FT-IR) spectrum of water correspond to vibrational transitions of the H_2O molecule, which are directly related to hydrogen bonding and molecular dynamics. Specifically, for the presented spectrum:

Region 3100–3600 cm^{-1} – O–H vibrations

This is the most characteristic region of water. The broad band arises from stretching vibrations of the O–H bonds. The width and shape of the Analemma Water reflect strong hydrogen bonding. The presence of different local environments (free and hydrogen-bonded O–H groups) is observed. This region indicates a structured hydrogen-bond network.

Conclusions

The obtained results show measurable differences between the Analemma Water sample and the control sample. In the NMR analysis, a difference in chemical shift was observed: the signal of Analemma Water was recorded at $\delta = 4.268$ ppm, while that of the control sample was recorded at $\delta = 4.217$ ppm. The difference, $\Delta\delta = 0.051$ ppm, indicates changes in the local molecular environment of the water protons. In addition, the difference

$\Delta\nu_{1/2} = 8.37 - 6.21 = 2.16$ Hz shows differences in the dynamics of molecular interactions.

The FT-IR analysis confirms that the 3100–3600 cm^{-1} region, characteristic of O–H vibrations, is particularly important for evaluating hydrogen bonds in water. The shape and width of this spectral region can be associated with different local environments of water molecules and with the possible presence of water cluster structures. The presented model indicates a more pronounced role of clusters composed of two (dimer), three (trimer), four (tetramer), five (pentamer), and six (hexamer) water molecules, suggesting dynamic restructuring of the hydrogen-bond network.