



Finding Water Molecules with Important Biological Activity

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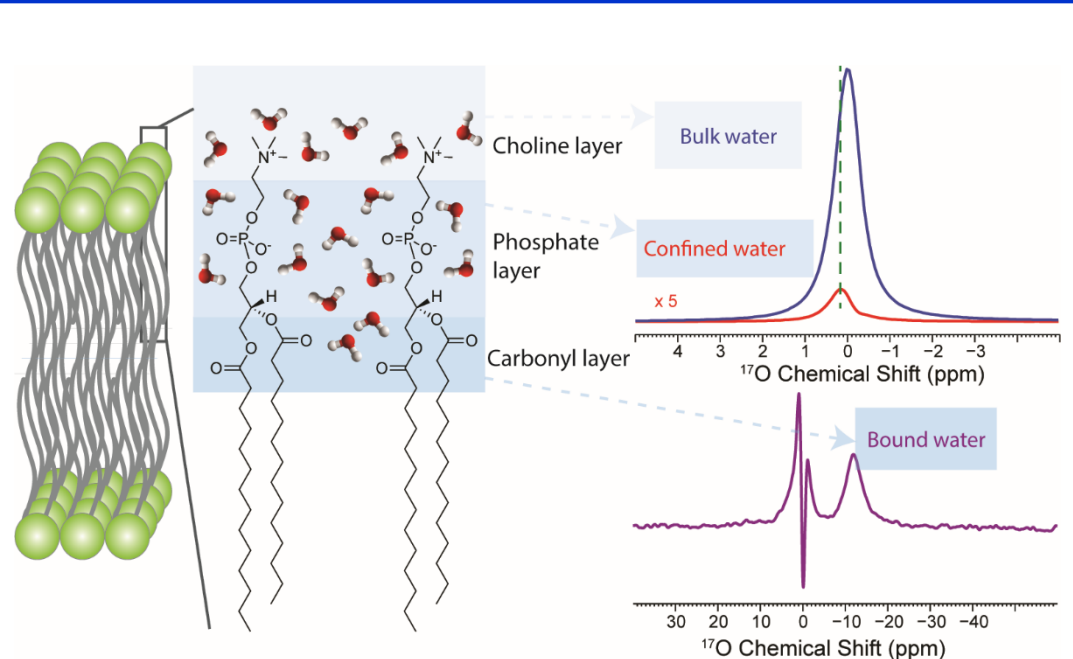
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Understanding the structures and dynamics of water molecules in biological systems, such as proteins and membranes, is crucial for addressing many problems in biology and medicine. To date, a direct NMR probe of “bound” water molecules in proteins and membranes has been evasive, largely because their signals are obscured by those of highly-mobile “bulk” water molecules.

Researchers have developed a novel ^{17}O solid-state NMR technique, in combination with the highest-field NMR magnet in the world (35.2T, Series-Connected-Hybrid, SCH) and ^{17}O -enriched water, to selectively suppress the dominant bulk water signals and allow for the direct detection of the bound water signals in an extensively hydrated lipid bilayer environment.

With this new approach, two chemically and dynamically distinct water species in the headgroup region of hydrated dimyristoylphosphatidylcholine (DMPC) lipid bilayers are identified for the first time. These interfacial water molecules are relatively stable for time periods on the order of milliseconds, providing an opportunity to characterize water dynamics on the millisecond or longer timescales in biomacromolecules of great biological significance.



Left: Molecules in the lipid bilayer under study. The hydration of the headgroup region is highlighted with different blue background shading reflecting the waters that interact with the choline, phosphate and carbonyl groups of the lipid headgroups.

Right: The ^{17}O NMR resonances of individual “bound” water molecules that are located in different layers of the lipid headgroup region, made visible using the 35.2T Series Connected Hybrid magnet system, even in the presence of much larger numbers of “bulk” water molecules.

Facilities and instrumentation used: NMR/MRI Facility: NHMFL 18.8T/800 MHz; DC Facility: 36T SCH.

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