Structure and Dynamics of Glassy, Supercooled and Nanoconfined Fluids
WORKSHOP 2019
Buenos Aires | Argentina | July 14 –16

CONICET
UNSE Universidad Nacional de Santiago del Estero
CIBAAL

"Response of water behavior at the interphase of phospholipid matrixes assessed by FTIR"

A. S. Rosa[1*], E. A. Disalvo y [1] M. A. Frías[1] .
[1] Laboratorio de Biointerfases y Sistemas Biomimeticos-CIBAAL-UNSE-CONICET, Argentina
*sebarosa007@hotmail.com

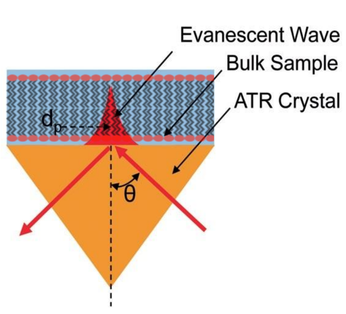
Introduction

Lipid membranes are one of the most important biological matrixes in which biochemical processes take place. This particular lipid arrangement is driven by different water disposition interacting with it, which is related to different water states with different energy levels at this interphase.

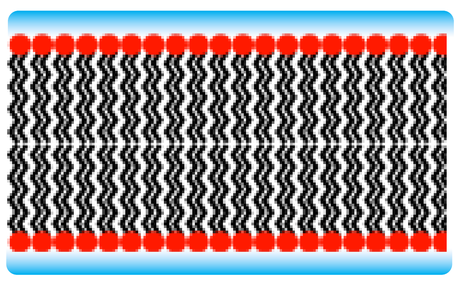
In our work, we report changes in water content and distinctive water states by FTIR when this self assembled matrix changes its physicochemical properties. The -OH stretching band in the liquid water IR spectrum is the principal region used to understand its molecular organization (4000-3000 cm^{-1}). The strength of the hydrogen-bonding depends on the cooperative/anti-cooperative nature of the surrounding hydrogen bonds, with strongest hydrogen bonds giving the lowest vibrational frequencies. Thus, we can use water as mirror of the membrane state in this kind of biological systems.[1,2]

Different phospholipids associate water at particular modes according to their structures; this may produce modulation of packing and hydration suitable for the incorporation of aminoacids, peptides and enzymes.[3]

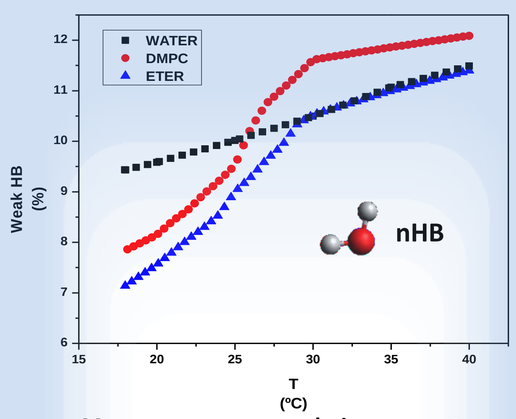
Results



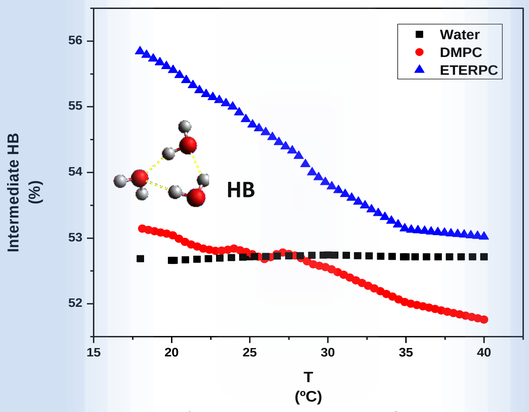
FTIR-ATR schematic representation . 2ul of lipid sample are placed on the diamond probe under controlled temperature



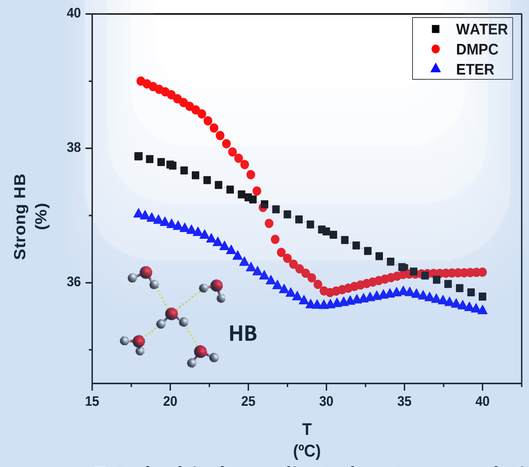
Water at the interphase of lipid bilayer shows different properties than bulk water



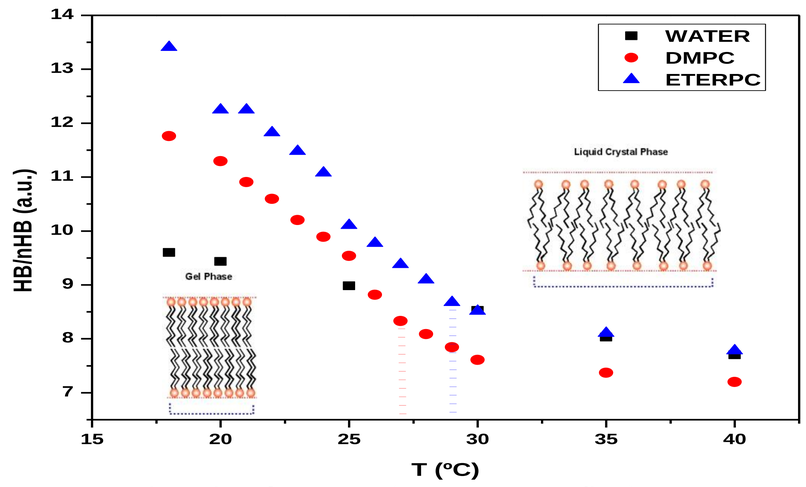
Monomer water population percent vs temperature . (3600 cm^{-1})



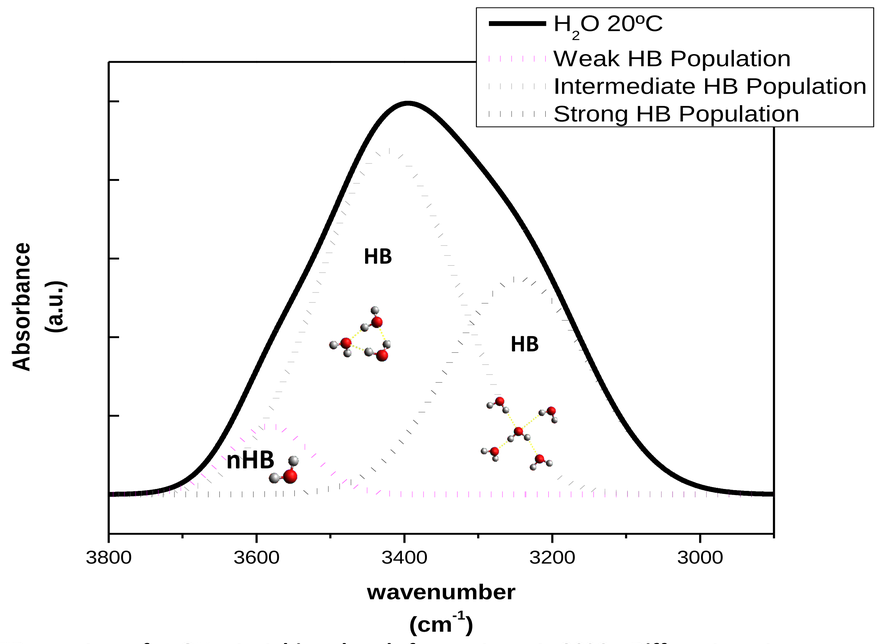
Intermediate HB water population percent vs temperature . (3400 cm^{-1})



Tetrahedrical coordinated water population percent vs temperature. (3200 cm^{-1})

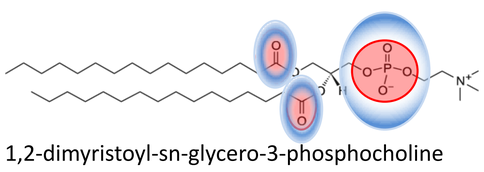


Intensity ratios of HB water (Strong + Intermediate) over Non HB water (Weak) vs temperature. A slope change is present at the lipid phase transition temperature.



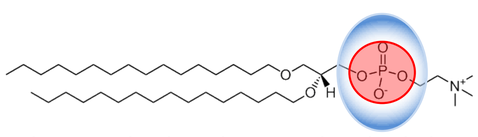
FTIR spectra of components are obtained by deconvolution and Gaussian curve fitting techniques.[1,2] **OH stretching band for water at 20ºC. Different water**

DMPC:

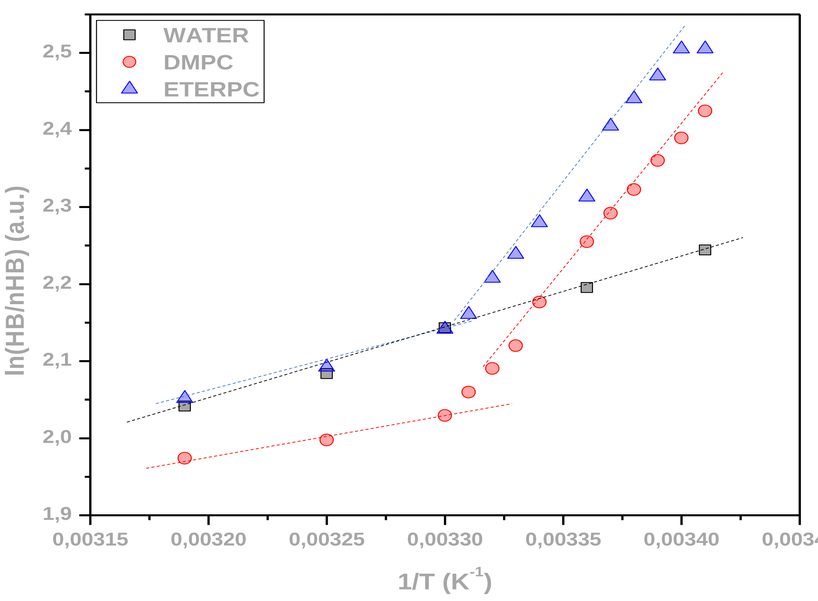


1,2-dimyristoyl-sn-glycero-3-phosphocholine

ETERPC:



1,2-di-O-tetradecyl-sn-glycero-3-phosphocholine



Enthalpy values of water hydrogen bonding calculated from Van´t Hoff equation.

ΔH (kcal/mol)	DMPC	ETERPC	WATER
Below Tm	**-7.4 ±0.4**	**-7.2±0.3**	**-1.9±0.1**
Above Tm	**-1.1 ±0.2**	**-1.6±0.2**	

Conclusion

- **Energy of Hydrogen bonds above Tm are similar to those in pure water. Below Tm Hydrogen bonds are much higher independently of the presence of carbonyl groups**
- **Water populations given by different H bonding arrangements are sensitive to lipid conformational states.**
- **Water rearrangements observed by FTIR gives information about Transition temperatures and water hydrogen bond enthalpy in lipid matrix systems.**

REFERENCES

1 De Ninno, A., Castellano, A. C., & Del Giudice, E. (2013). The supramolecular structure of liquid water and quantum coherent processes in biology. In *Journal of Physics: Conference Series*(Vol. 442, No. 1, p. 012031). IOP Publishing.
2 Freda, M., Piluso, A., Santucci, A., & Sassi, P. (2005). Transmittance Fourier transform infrared spectra of liquid water in the whole mid-infrared region: temperature dependence and structural analysis. *Applied spectroscopy*, *59*(9), 1155-1159.
3 Disalvo, E. A., & Frias, M. A. (2013). Water state and carbonyl distribution populations in confined regions of lipid bilayers observed by FTIR spectroscopy. *Langmuir*, *29*(23), 6969-6974.