

# XLVIII Reunión Anual de la Sociedad Argentina de Biofísica

Libro de Resúmenes



**SAB**  
XLVIII

27 al 29 de noviembre de 2019  
Universidad Nacional de San Luis

XLVIII Reunión Anual de la Sociedad Argentina de Biofísica / compilado por  
Sebastián Andujar ...  
[et al.]. - 1a ed. - Buenos Aires : SAB - Sociedad Argentina de Biofísica, 2019.  
Libro digital, PDF

Archivo Digital: descarga  
ISBN 978-987-27591-7-9

1. Biofísica. 2. Investigación. I. Andujar, Sebastián, comp.  
CDD 570

### *Diagramación y Edición*

M. Soledad Celej, Juan Pablo Acierno

### *Diseño de Tapa y Logo*

Comité Organizador

### *Asistencia Técnica Web*

Juan Pablo Acierno

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**XLVIII Reunión Anual SAB**

**27-29 Noviembre 2019**

**San Luis, Argentina**

**XLVIII Annual Meeting SAB**

**27-29 November 2019**

**San Luis, Argentina**

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Aires

## Hydrogen bonds and water in steroid-containing phospholipidic membranes assessed by near infrared spectroscopy

**Wenz JJ<sup>a</sup>**

*a - Instituto de Investigaciones Bioquímicas de Bahía Blanca (INIBIBB). Departamento de Biología, Bioquímica y Farmacia, Universidad Nacional del Sur (UNS- CONICET), Bahía Blanca, Argentina*

Near infrared spectroscopy (NIR) is useful to study the H-bonds network in water systems, which are sensitive to solutes. The less the number and/or the strength of H-bonds, the more the strength of the covalent O-H bonds of water. Hence, they vibrate and absorb radiation at higher frequencies. By taking advantage of this spectral shift water in DMPA membranes with and without one of two steroids, progesterone and 25-hydroxycholesterol, was assessed.

Spectra of vesicles of DMPA and DMPA/steroid in MilliQ water (500  $\mu$ M; 80:20 molar ratio for the steroid-containing samples) between 1100 and 2300 nm were acquired at 10 temperatures in the range 13-58 °C, with a path length of 1 mm. For understanding the tangled spectra, principal component analysis was applied to disclose subtle changes mirroring the alterations in the vibrational energy of the O-H bonds, as an indirect measure of the H-bond network. The analysis encompassed the first overtone of water (centered at 1450/1455 nm) representing signals of overlapping water and O-H stretching bands, as well as a limited portion of 1100-1300 nm.

The shift to higher frequencies (i.e. higher energy) of the O-H vibration band with increasing temperatures or in the presence of 25-hydroxycholesterol is consistent with a strengthening of the O-H bonds caused by disruption/weakening of the H-bonds. The number of strongly H-bonded waters decreases whereas the number of weakly H-bonded waters increases. The observed shift agrees with reports about the distinct absorption of three states of water: waters having no -OH bonded, having one -OH group H-bonded and having two -OHs H-bonded. In contrast, DMPA and progesterone did not show significant effects on the H-bonds network. Findings concur with the lipid domain-promoting activity reported for 25-hydroxycholesterol (a cholesterol-like behavior) and with the slightly (or absent) lipid domain-disrupting activity of progesterone.