XLIX SAB 2021

XLIX Reunión Anual SAB

1 al 3 de diciembre 2021

Sociedad Argentina de Biofísica
XLIX Reunión Anual SAB / compilación de José María Delfino ... [et al.]. - 1a ed. - Ciudad Autónoma de Buenos Aires: SAB - Sociedad Argentina de Biofísica, 2021.
Libro digital, PDF

Archivo Digital: descarga y online
ISBN 978-987-27591-9-3

1. Biofísica. 2. Investigación Experimental. I. Delfino, José María, comp. II. Título.
CDD 571.4

Diagramación y Edición

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Member of the International Union for Pure and Applied Biophysics

XLIX Reunión Anual SAB

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Argentina

XLIX Annual Meeting SAB

1-3 December 2021

Argentina

Gabaergic insecticides exploration: interaction with biological membranes. An experimental and *in silico* approach.

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The study of many insecticidal compounds includes the knowledge of their interaction with a specific receptor protein under the ligand-receptor model. However, considering membrane receptors and mainly to lipophilic ligands, this interaction can be non-specifically modulated by changes in the physical properties of the membrane, due to the activity of these same products on the surrounding lipid molecules modulating the supramolecular organization of the receptor environment. The objective of this work is to describe how the lipophilic gabaergic insecticide Fluralaner affects the biophysical properties of DPPC Langmuir monolayers used as model membranes. We analyzed these effects by experimental and *in silico* complementary approaches. Experimental penetration isotherms indicated that the Fluralaner can be absorbed into the monolayer. Langmuir compression isotherms showed that Fluralaner molecules produce an expansion in the DPPC isotherm, by acting as spacers between the phospholipids. Also, the partition of Fluralaner molecules into the lipidic phase affects the characteristic DPPC phase transition, making it occur at higher surface pressure values. To provide a molecular insight into the behavior of the system, we performed ALL ATOM detail Molecular Dynamics simulations of DPPC monolayers in the presence of Fluralaner at different molecular packing states of the phospholipid. We were able to determine the probable distribution of Fluralaner at different regions of the DPPC monolayer and to observe an expansion of the simulated DPPC compression isotherm in the presence of Fluralaner, as observed experimentally. We are currently performing a series of umbrella sampling simulations to compute the potential of mean force (PMF).This will allow us to gain a thermodynamic insight on the partition of the insecticide into the lipidic phase.

Acknowldegments

This work was supported by grants from SECyT-UNC, FONCyT and CONICET.