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BLM21_Insertion of Glyphosate into a lipid bilayer: Study by molecular dynamics

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Herbicides are very useful for agriculture, allowing the elimination of weeds for the optimum development of crops. In the last decades, glyphosate has been the most widely used herbicide in the world. Currently, it is used without an accurate knowledge of its adverse effects on human health. Independent studies have shown that the glyphosate present some toxicity in laboratory animals [1-3]. In order to understand how the glyphosate interacts with a cell, in a first approximation, we model the process of insertion of this herbicide molecule into a lipid bilayer, using the molecular dynamics technique. The main goal is to determine the precise location of the glyphosate within the membrane, determining the free energy profiles of this process [4,5].

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BLM22_To Be Or Not To Be In Membrane Domains: Transbilayer Asymmetry And Sphingomyelin-Dependent Preferential Partitioning Of The Acetylcholine Receptor

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The preferential partitioning of the nicotinic acetylcholine receptor (AChR) in liquid-ordered (Lo) domains, heterogeneous membrane domains commonly known as rafts,is thought to be a part of its clustering mechanism. Previous studies from our group have shown that AChR lacks preference for Lo domains when reconstituted in sphingomyelin (SM), cholesterol (Chol) and POPC (1:1:1) model systems. Here we study the effect on the possible Lo-preferential partitioning of purified AChR reconstituted in two model systems (POPC:Chol, 1:1 and POPC:Chol:SM, 1:1:1) under: a) induced transbilayer asymmetry, by addition of brain sphingomyelin (bSM) to the external hemilayer; and b) the presence of different pure SM species in the model membrane (bSM, 16:0-SM, 18:0-SM or 24:1-SM). AChR distribution was evaluated by fluorescence resonance energy transfer efficiency between the AChR intrinsic fluorescence and Laurdan or dehydroergosterol fluorescence, and also by determining the presence of AChR in detergent-resistant and detergent-soluble domains (1% Triton X-100, 4°C). Both studies show that the induction of transbilayer asymmetry or the presence of 16:0-SM or 18:0-SM, as opposed to bSM or 24:1-SM, leads to a preferential partitioning of AChR in Lo domains. Thus, the localization of AChR in Lo domains strongly depends on the characteristics of the host lipid membrane.