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In silico study of lipids associated in non-bilayer phospholipid arrangements

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Statement of the Problem: Systemic lupus erythematous (SLE) is an autoimmune, chronic and multifactorial disease. For SLE study, some animal models had been developed, and our lab has one. Our model was obtained by administering a different lipid bilayer structure called non-bilayer phospholipid arrangements. These non-bilayer phospholipid arrangements can be stabilized with drugs such as chlorpromazine or procainamide and specifically in female mice, causing a disease very similar to human SLE. To help understand how these lipid structures in the development of the disease involved, we used bioinformatics tools to understand how they form, and now we'll try to extrapolate this to explain some of the symptoms faced by patients with SLE.

Methodology & Theoretical Orientation: A molecular simulation was established using all the conditions used in our murine model with chlorpromazine and was created with GROMACS software. Analyses of results were made with GROMACS utilities, proprietary Python programs and VMD tools.

Findings: With our simulation strategy, we were able to observe differences between diverse lipidic environments with one or various molecules of chlorpromazine. Also, we have started new simulations to improve our strategy and get more useful information for our molecular knowledge of the models and the etiology of the human disease.

Conclusion & Significance: These findings help us to understand how the models are triggered and give us clues about how to improve them for a further research of how SLE is initiated in humans. That probably will contribute to the improvement of the models and support our novel theory about the etiology of the SLE disease in humans.

Biography

Sánchez B Sandra has her expertise in Molecular Biology and Bioinformatics, and is passionate about Biochemistry and Science Communication. Her novel approximation to the function of a drug on a bilayer membrane can help to better understand our murine models and how this can impact our knowledge on the systemic lupus erythematosus disease. She has built her abilities after years of experience in research, project administration and protocols development in the Pharmaceutical Industry, teaches of Biochemistry and Genetics for physicians, and translates pharmaceutical documents and participates in science fairs for kids. This work was possible due to her willingness to collaborate with external researchers, as Laura Domínguez from FQ-UNAM and Cornelio Yañez from CIC-IPN, who gave her the tools and knowledge to use bioinformatics and a Mexican Supercomputer to realize this project.

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