



# **SIMULACIÓN MOLECULAR EN CÁNCER, INFECCIÓN Y ENVEJECIMIENTO: UN MICROSCOPIO VIRTUAL PARA EL DISEÑO DE NUEVAS TERAPIAS**



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Jornada de Usuarios CESGA 2023



PID2022-141534OB-I00



PDC2022-133402-I00



PID2019-111327GB-I00



**XUNTA  
DE GALICIA**



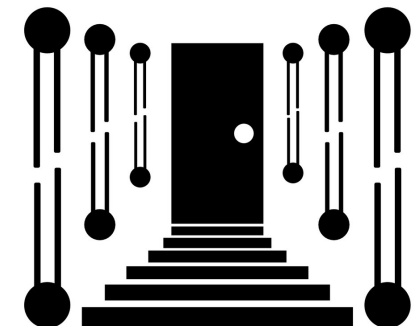
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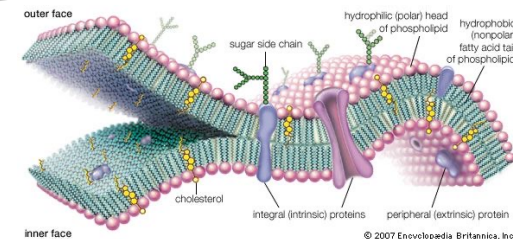
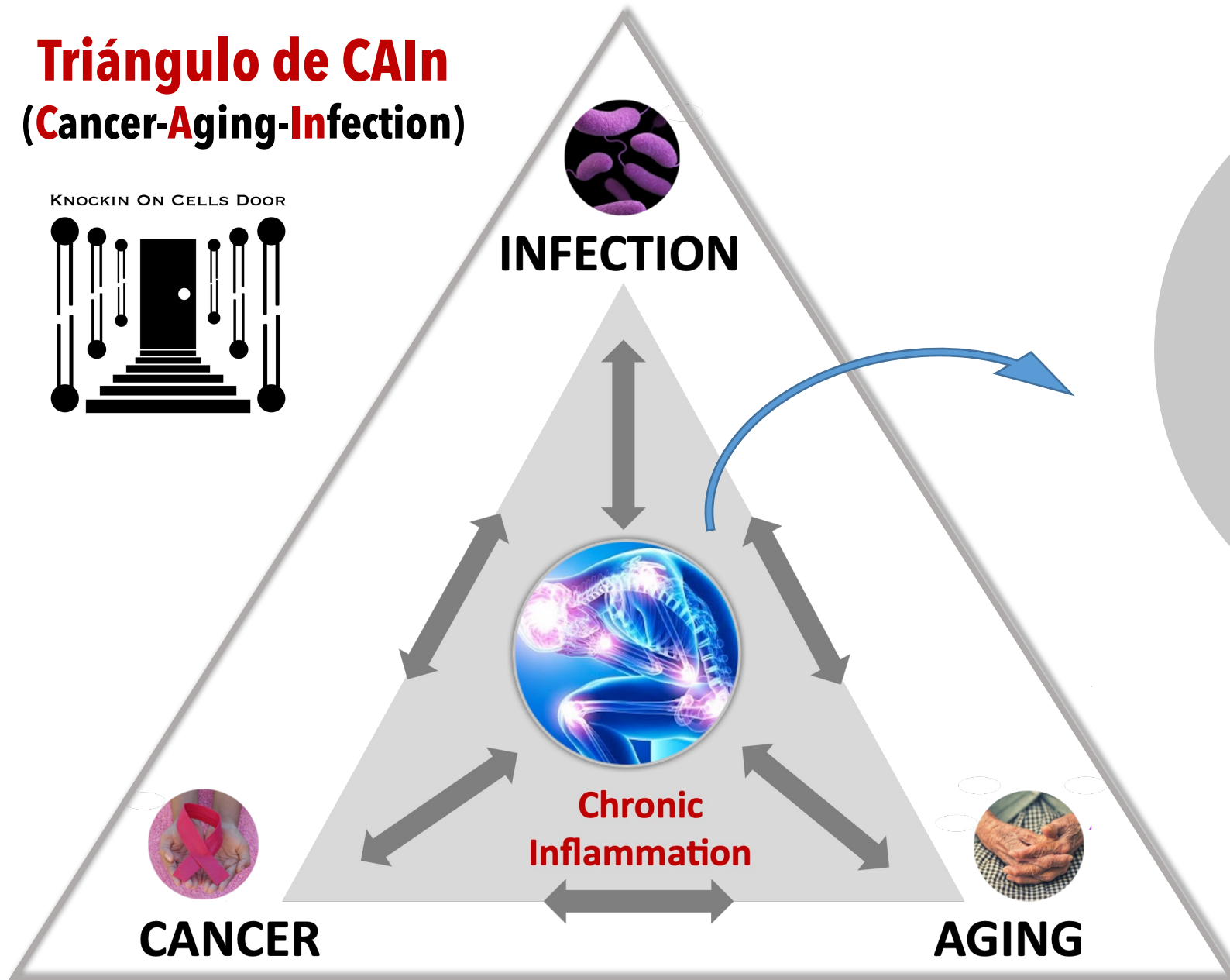
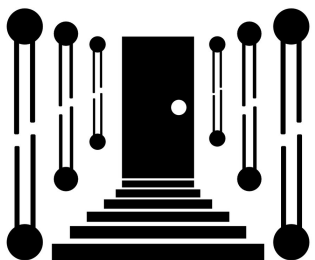
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Paula Antelo Riveiro

César Porto Vence

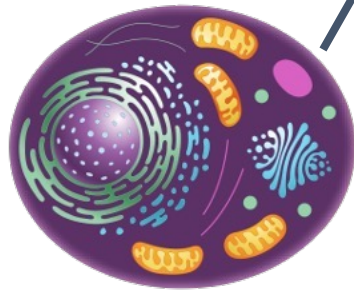
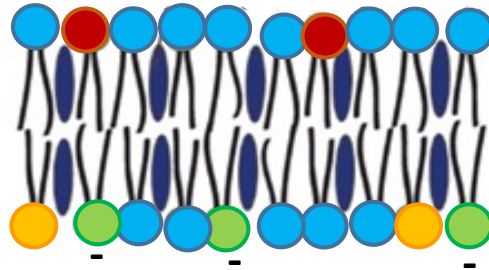
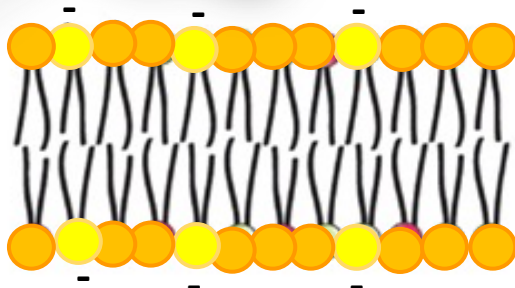
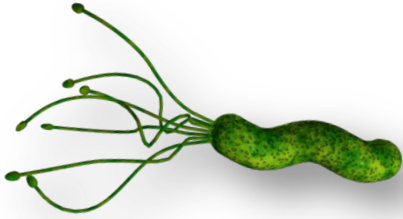
## Triángulo de CAIn (Cancer-Aging-Infection)

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Conde-Torres; D. Blanco-González, A.; Cabezón, A.; Suárez-Lestón, F.; Seco-González, A.; Antelo, P.; Piñeiro, Á.; Garcia-Fandino, R. "The CAIn Triangle: Deciphering the Interconnections between Cancer, Aging, and Infection through Inflammation and Lipid Composition", **2023**, *enviado*.

**Bacteria**



**Mamífero sano**



**Envejecimiento**

PG



PC



PS



PE



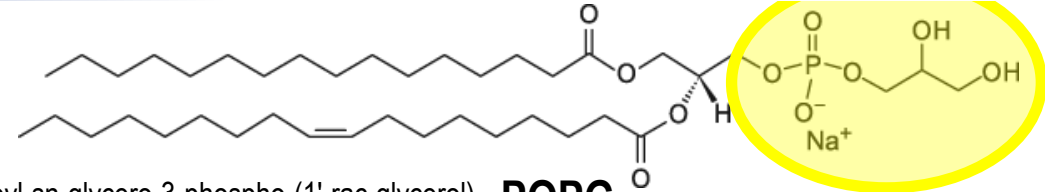
SM



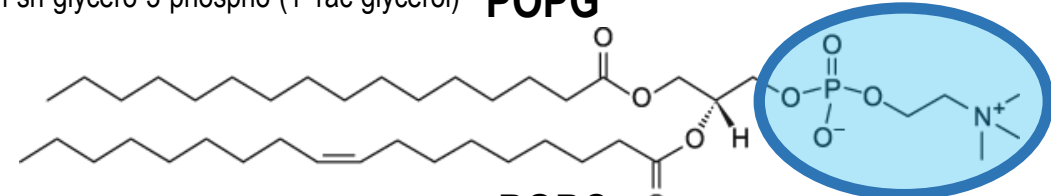
Chol



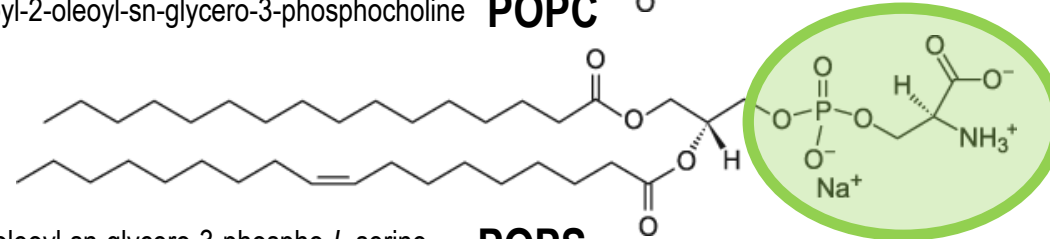
1-palmitoyl-2-oleoyl-sn-glycero-3-phospho-(1'-rac-glycerol) **POPG**



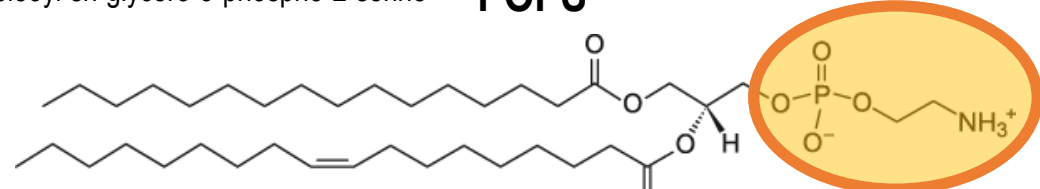
1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine **POPC**



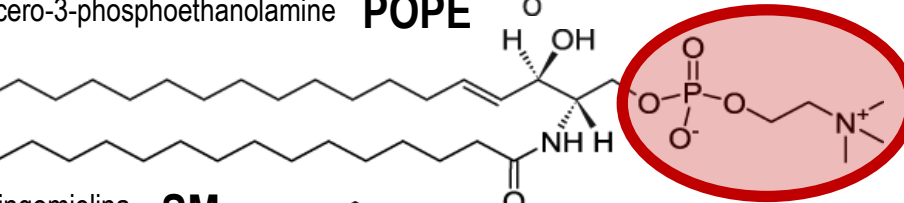
1-palmitoyl-2-oleoyl-sn-glycero-3-phospho-L-serine **POPS**



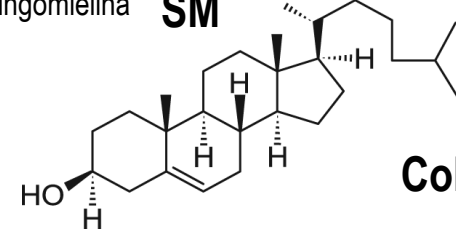
1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine **POPE**



Esfingomielina **SM**



**Colesterol**



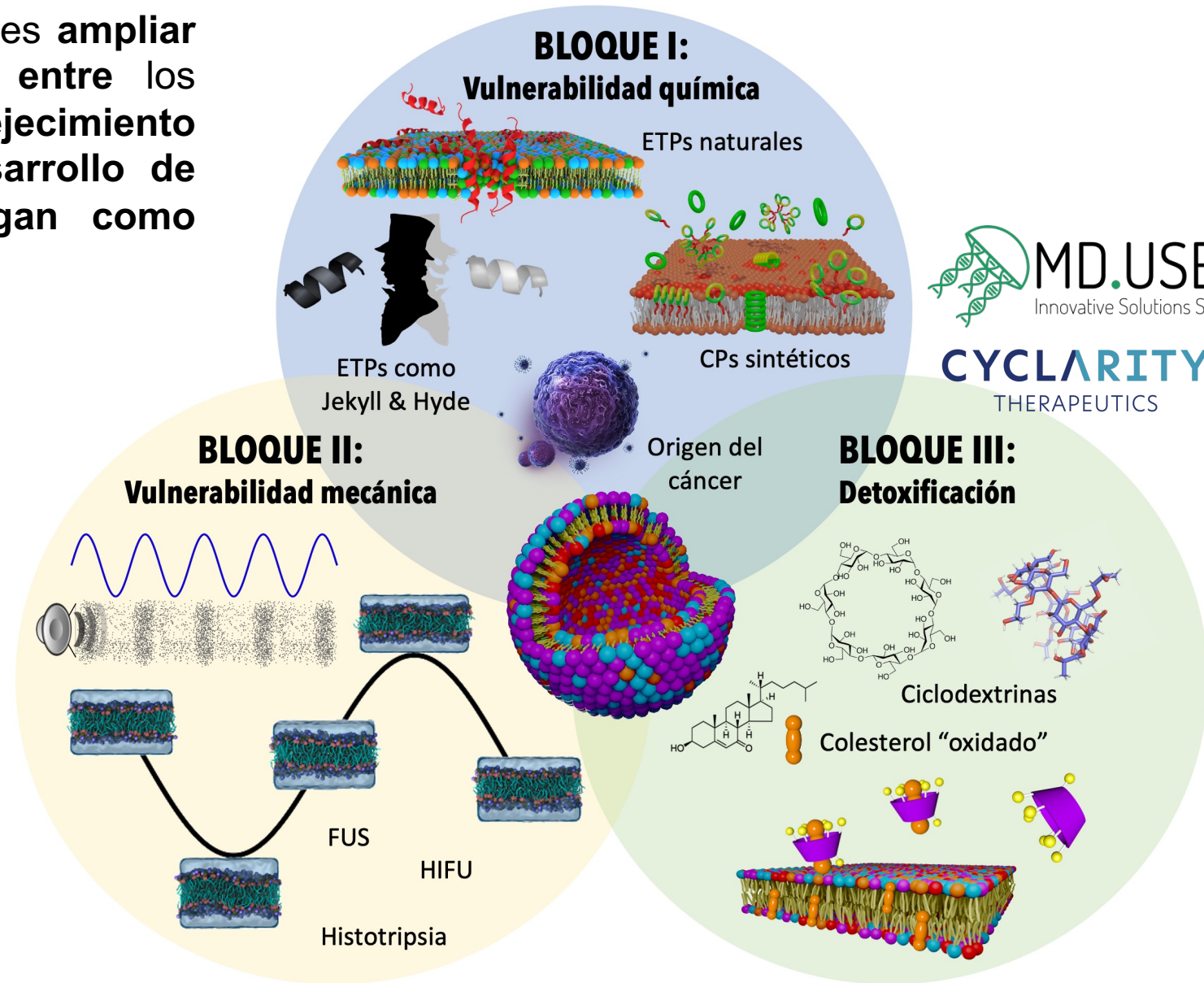
El **objetivo principal** de nuestra investigación es ampliar nuestra comprensión sobre la conexión entre los elementos del triángulo de CAIn (**cáncer, envejecimiento e infección**) con el fin de contribuir al desarrollo de nuevas estrategias terapéuticas que tengan como diana la membrana celular.

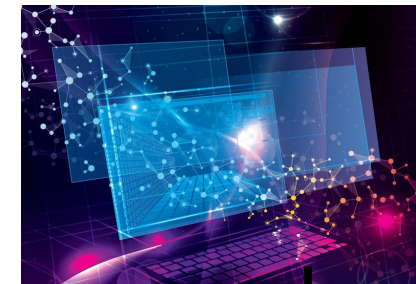
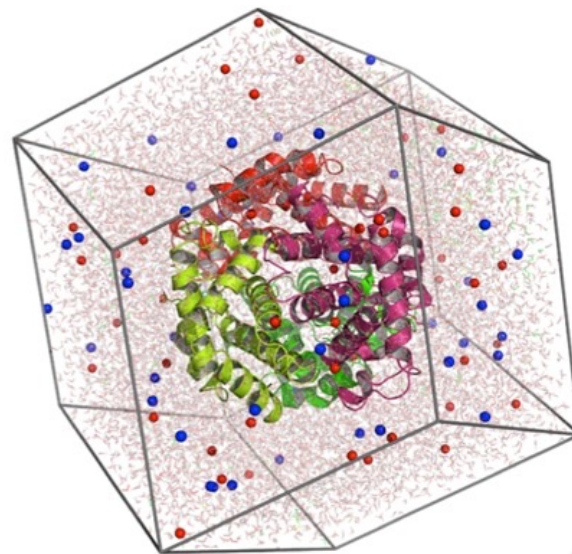
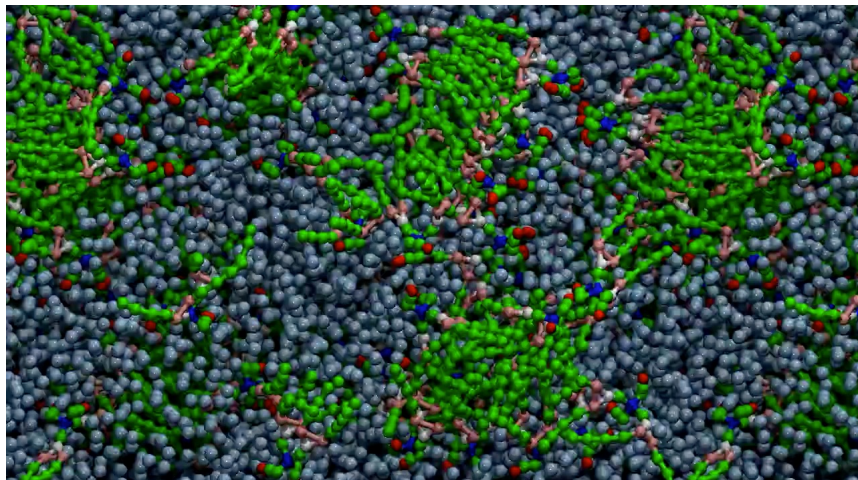
## Objetivos específicos:

Identificar las vulnerabilidades fisicoquímicas de las membranas lipídicas para tratar de destruirlas mediante péptidos lineales y cíclicos (**Bloque I**)

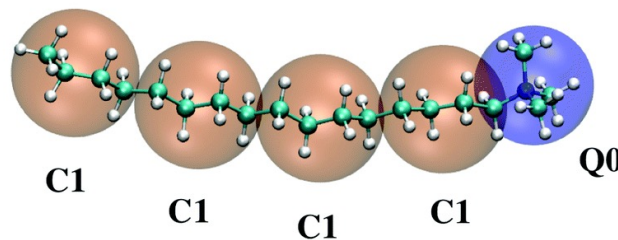
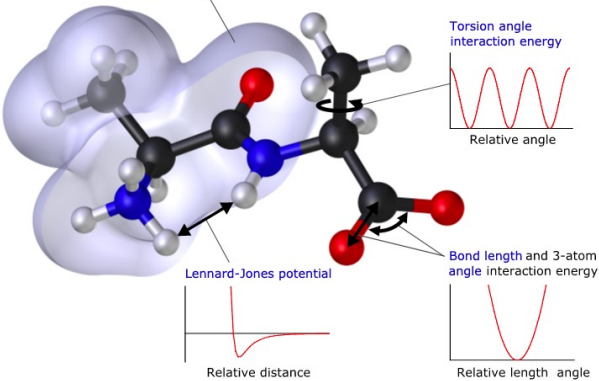
Identificar vulnerabilidades mecánicas de las membranas en función de su composición lipídica y evaluar su respuesta a perturbaciones externas (**Bloque II**)

Desarrollar estrategias de reparación de la membrana a nivel de composición lipídica, utilizando principalmente derivados de ciclodextrinas (**Bloque III**)





Hydrophobic effect is approximately proportional to surface area



Resolución atomística (AT) /  
Coarse-Grained (CG)

Campo de fuerzas

**Lipidómica**

**Monocapas lipídicas**

**Bicapas lipídicas**

**Liposomas**

**Dinámica Molecular**

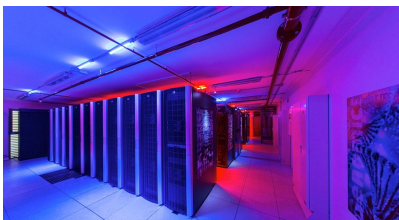
**Análisis Big Data**

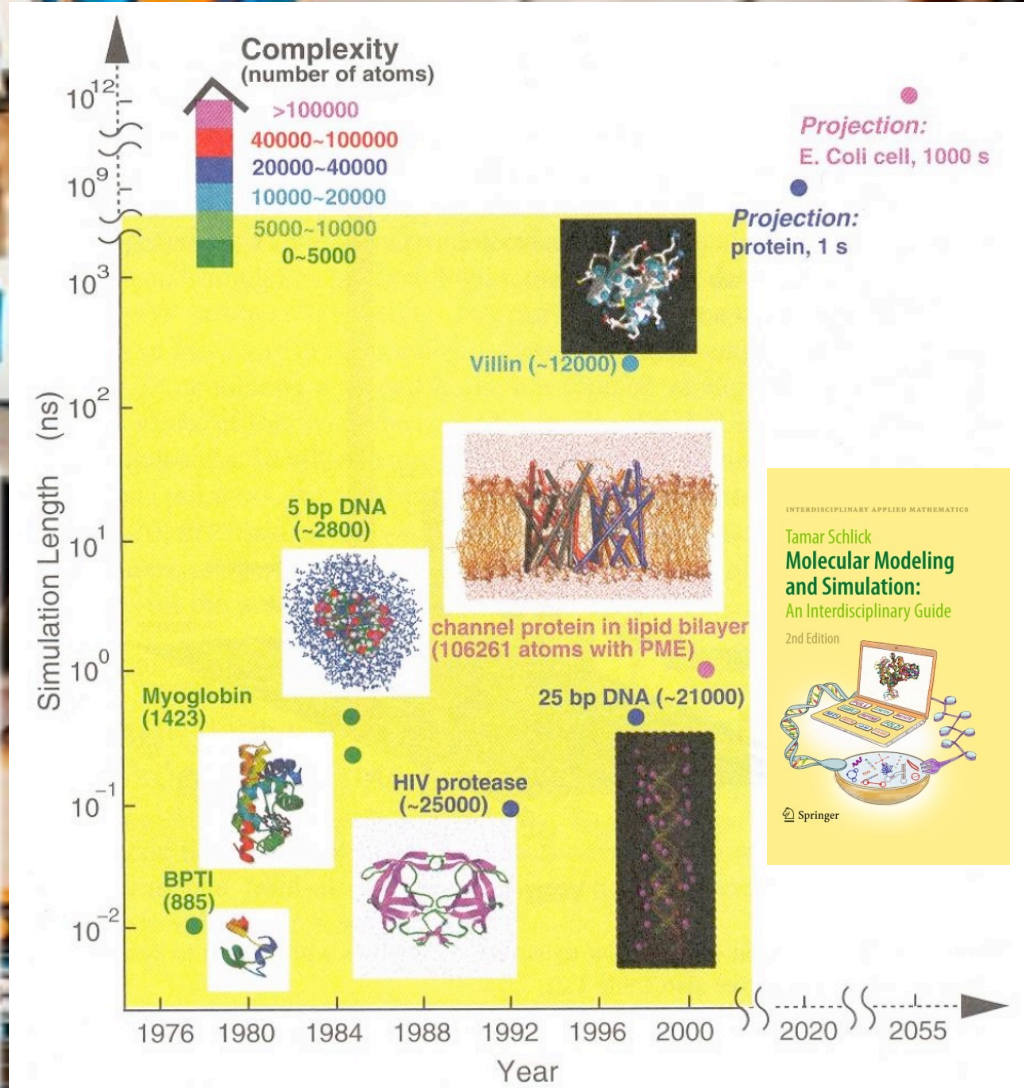
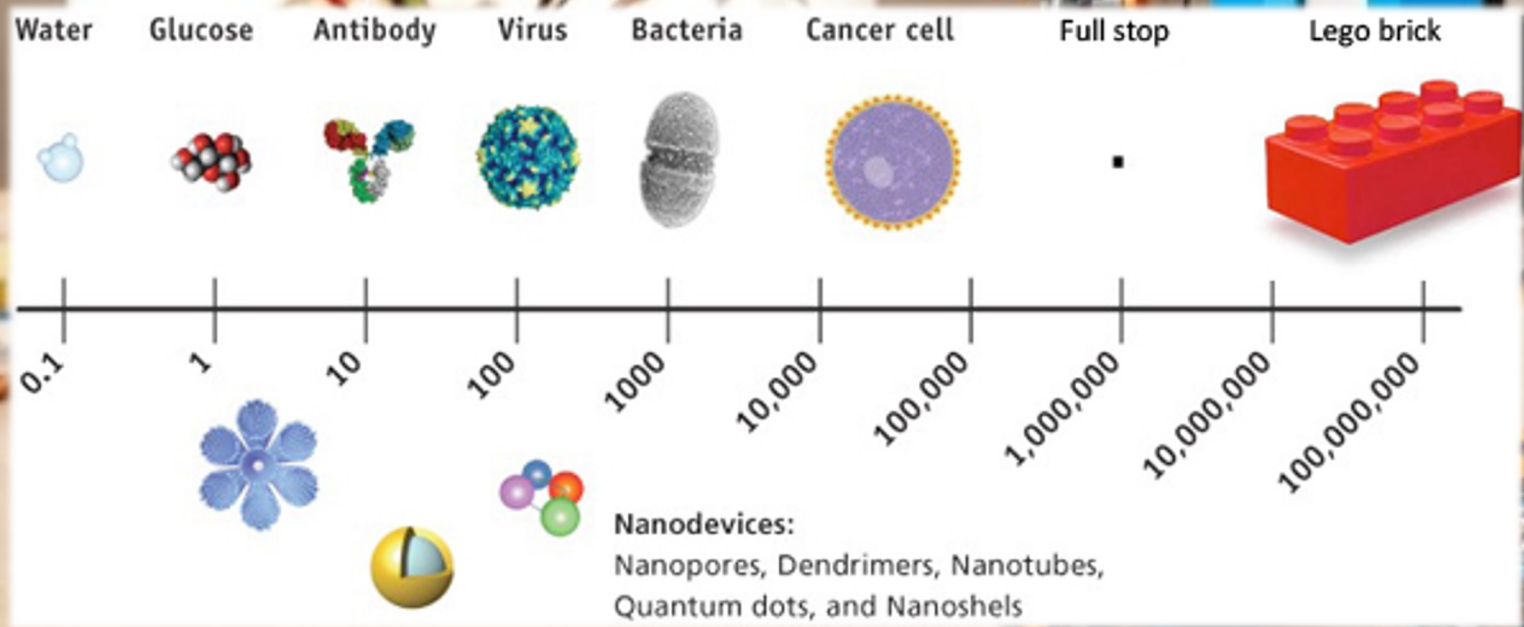
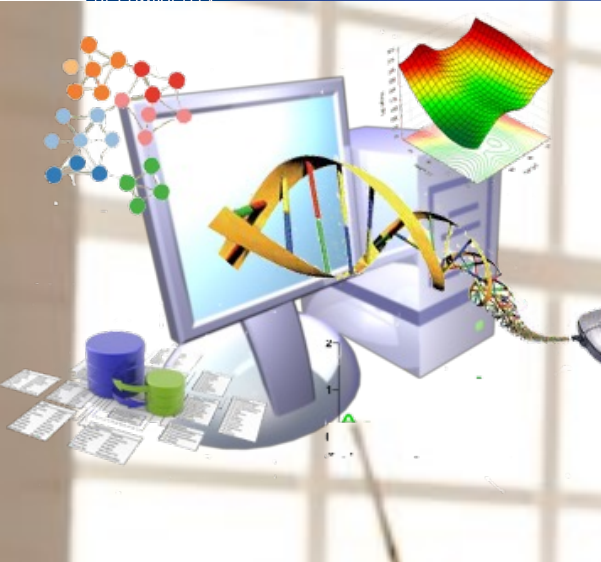
**Machine Learning**

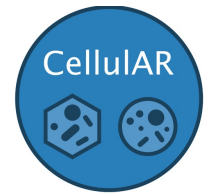
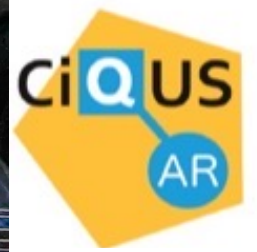
**Computación cuántica**

**Experimentos biofísicos**

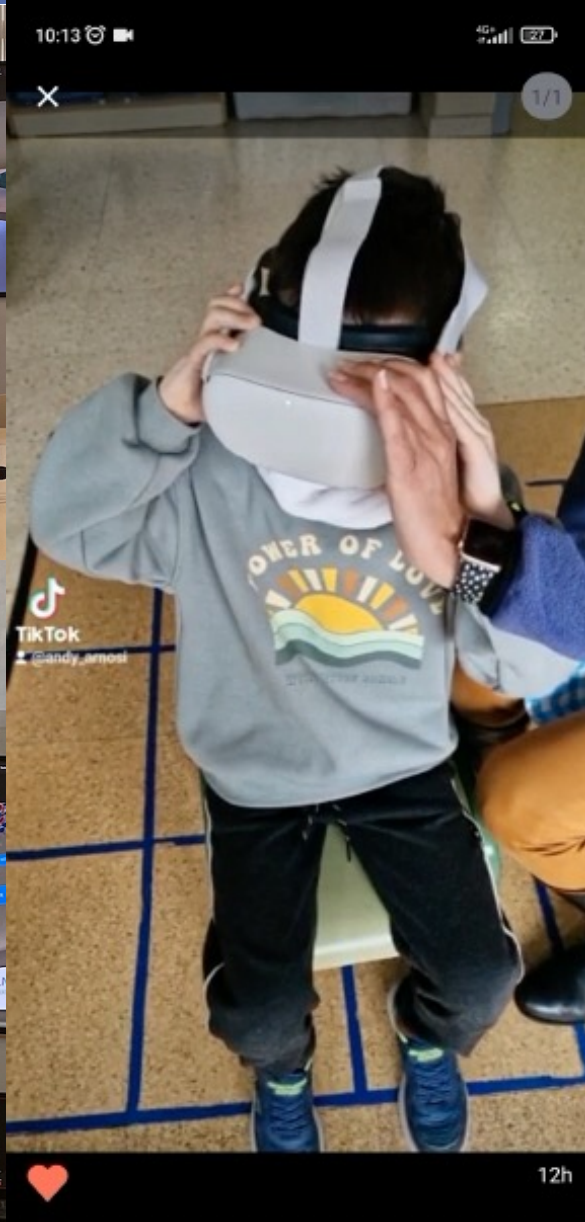
**Aproximación computacional**













**GRACIAS POR LA ATENCIÓN!!**