THE OMG APPROACH: A USER-FRIENDLY MOLECULAR SIMULATION TOOL FOR MEMBRANE DYNAMICS

Bozdaganyan M., Orekhov P., Yang A.

Shenzhen MSU-BIT University, 1 International University Garden Road, Dayun New City,Longgang District, Shenzhen City, Guangdong Province, 518172, China
+86-15816878293, m.bozdaganyan@gmail.com

The simulation of membrane systems poses a significant challenge due to the intricate structure of mixed lipid bilayers and the dynamic nature of molecular-lipid interactions. To address this, we introduce a novel molecular simulation tool, the OpenMM-Google Colab set (OMG), which combines OpenMM and Google Colab. This integration enables seamless molecular simulations and collaborative data analysis, eliminating the need for extensive expertise in the field. Using the OMG tool, we investigate the potential of mean force (PMF) between the skin cell membrane and different hydrophilic, hydrophobic, and neutral beads, represented using the MARTINI notation. By equilibrating the membrane at 310 K for 0.5 microseconds, we explore the molecular behavior within the system. Additionally, we estimate the logarithm of the partition coefficient (logKp) by adopting an approach similar to [1].Expanding our analysis, we calculate PMFs and logKp values for selected compounds sourced from the CPE DB [2]. Our findings demonstrate the capability of the OMG tool in accurately predicting the permeability of Martini singular bead and dimer beads within a membrane comprising ceramide, cholesterol, and free fatty acid in a 1:1:1 ratio. These results align remarkably well with experimental data, exhibiting a high R-square value of 0.8. This research holds immense promise as a valuable resource for the development and screening of chemical compounds intended for transdermal drug delivery. By offering a user-friendly platform for membrane simulation, the OMG tool has the potential to revolutionize the field of membrane dynamics research.

References.

1. Hoffmann, C., Centi, A., Menichetti, R. et al. Molecular dynamics trajectories for 630 coarse-grained drug-membrane permeations. // Sci Data 7, 51 (2020).
2. Vasyuchenko, E. P., Orekhov, P. S., Armeev, G. A. & Bozdaganyan, M. E. CPE-DB: An Open Database of Chemical Penetration Enhancers. // Pharmaceutics 13, 66 (2021).