

**Annual highlight** Scrima S, et al. *Comput Struct Biotechnol J*, 2022

Cell membranes are barriers that define the boundaries of cells or of different compartments in the cell (subcellular membranes). They are "borders" that control the flux of material, including drugs, and information between compartments and are very important for several cellular functions. Membranes are mostly made of a mixture of lipids (fats), which vary from membrane to membrane. Importantly, changes in their composition have been linked to cancer. Membranes also host specific proteins, cellular actors that carry out specific functions in the cell and whose performance and behavior depend on the membrane they are embedded in. Unfortunately, we don't have much information about the precise makeup of these subcellular membranes, and we don't know how this influences their function. To better understand how membrane composition contributes to cellular processes and cancer, we researchers at CARD are using a combination of experiments and computer simulations. Experiments inform us about the types of lipids different membranes are made of, while simulations can be used to probe the fine, small-scale details of the consequences that the composition has on the shape, thickness, and other properties of cellular membranes. This helps us understand in what way membranes differ between healthy and cancerous cells or in the presence of drugs. In this context, we have developed a software called LipidDyn, to help us make the best out of our simulations. LipidDyn helps us in two significant ways. First, it improves our ability to design computer simulations of cellular membranes with specific compositions so that we can simulate different types of membranes or membranes from healthy or cancer cells. Second, we use it to make sense of our simulations and extract relevant information from them on how our membranes behave in the simulation. For instance, LipidDyn can tell us about the shape, thickness, rigidity, or how curved our membrane is. These properties are important to understand how lipid composition influences the behavior of membranes. We can also use LipidDyn to monitor how the membrane and its embedded proteins influence each other. For example, we have used LipidDyn to investigate: i) the effects of cancer drugs on lysosomal membranes and enzymes; ii) the changes in membranes associated with dietary lipids; and iii) the lipid-transport mechanisms that control the shape and composition of membranes. LipidDyn is in active development and freely available; if you're curious to have a look at our code, you can explore it at <https://github.com/ELELAB/LipidDyn>.

