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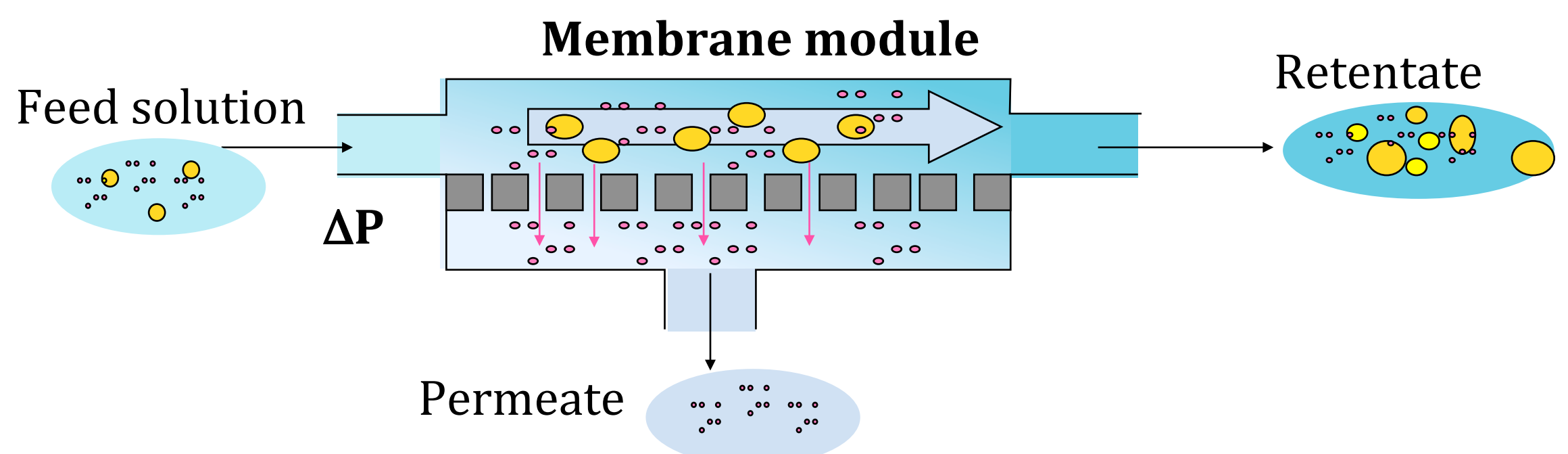
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Lipids behaviour in aqueous solution of disrupted microalgae : molecular simulation of representative synthetic mixtures

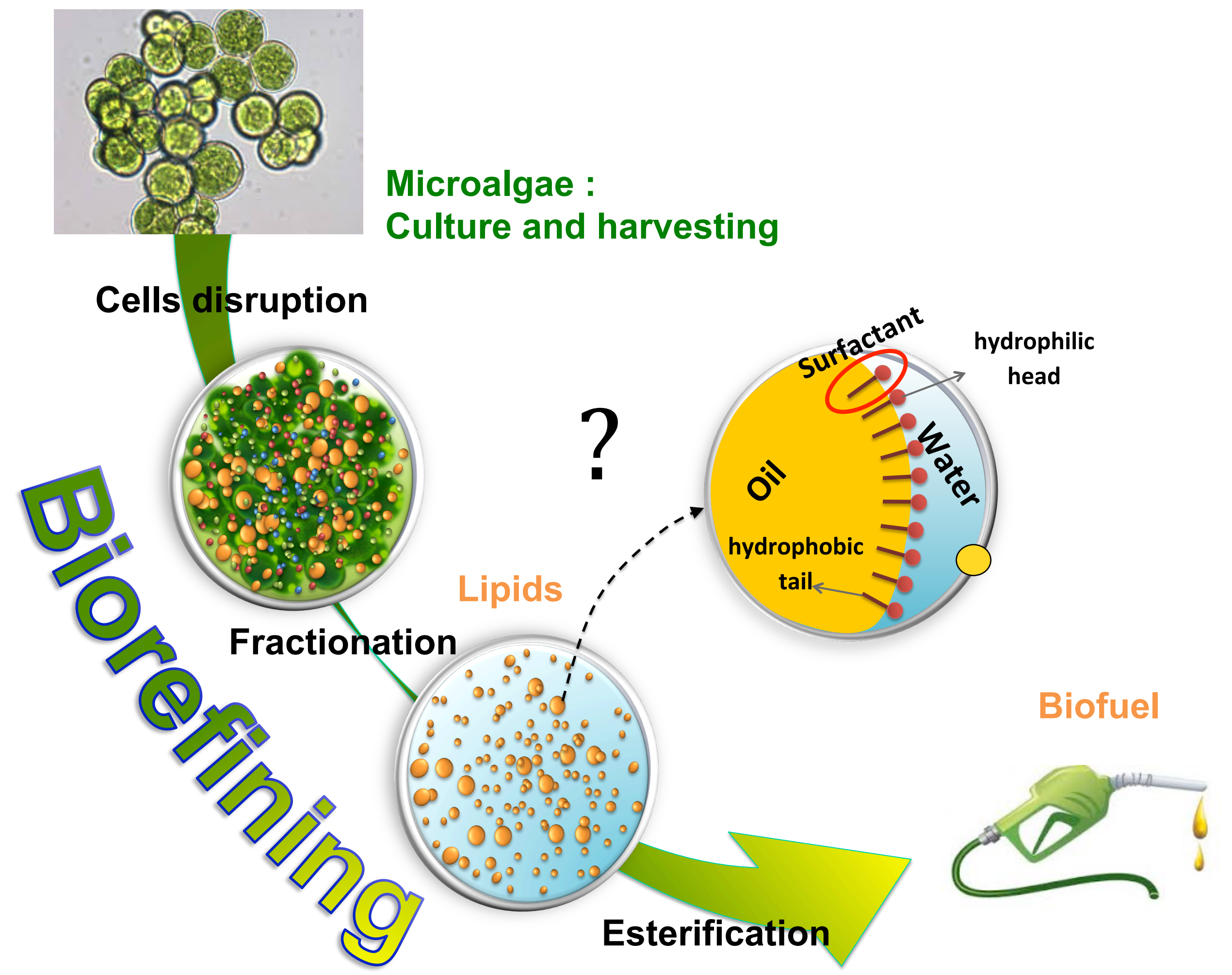
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Context

The use of microalgae for the production of biofuels and renewable feedstocks is an extremely promising sustainable technology. However, there are still challenges for its large scale implementation. **The harvesting and extraction steps are two main areas of improvement.** Harvested microalgae have to be grinded and lipids extracted, concentrated and purified. This downstream processing can be implemented by several processes within **membrane filtration**.



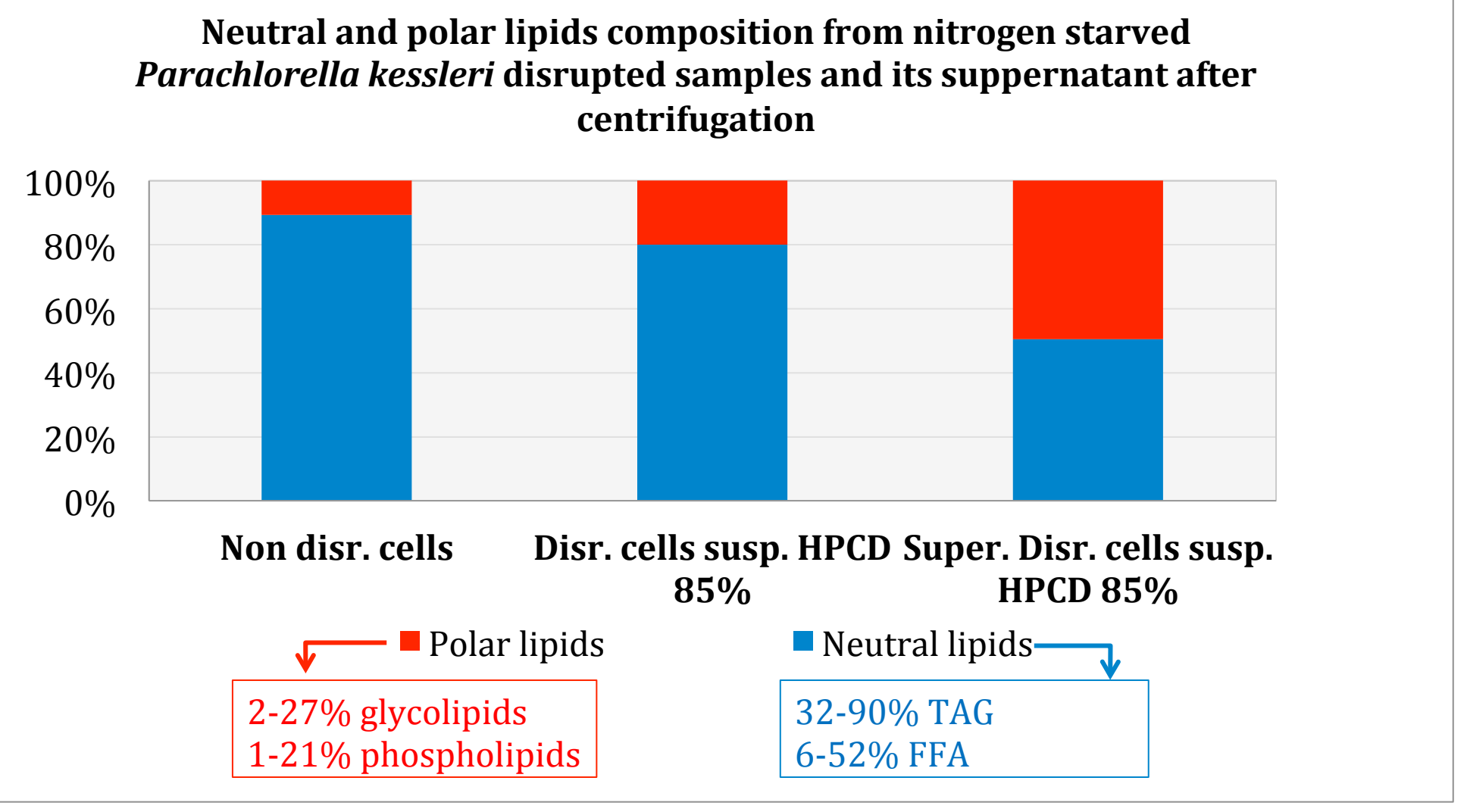
The **understanding of local organization of lipids** and valuable compounds in the complex solution and during the separation is a **great challenge to optimize the fractionation processes.** The Coarse-grained molecular dynamics simulation is a powerful tool to achieve this goal. **The first compounds that are studied at local scale are neutral lipids (triglycerides, free fatty acids)** produced by microalgae and biofuel precursor, polar lipids (phospholipids, glycolipids), and polymeric membrane (polyamide or polyethersulfone) used for separation.



Material and methods

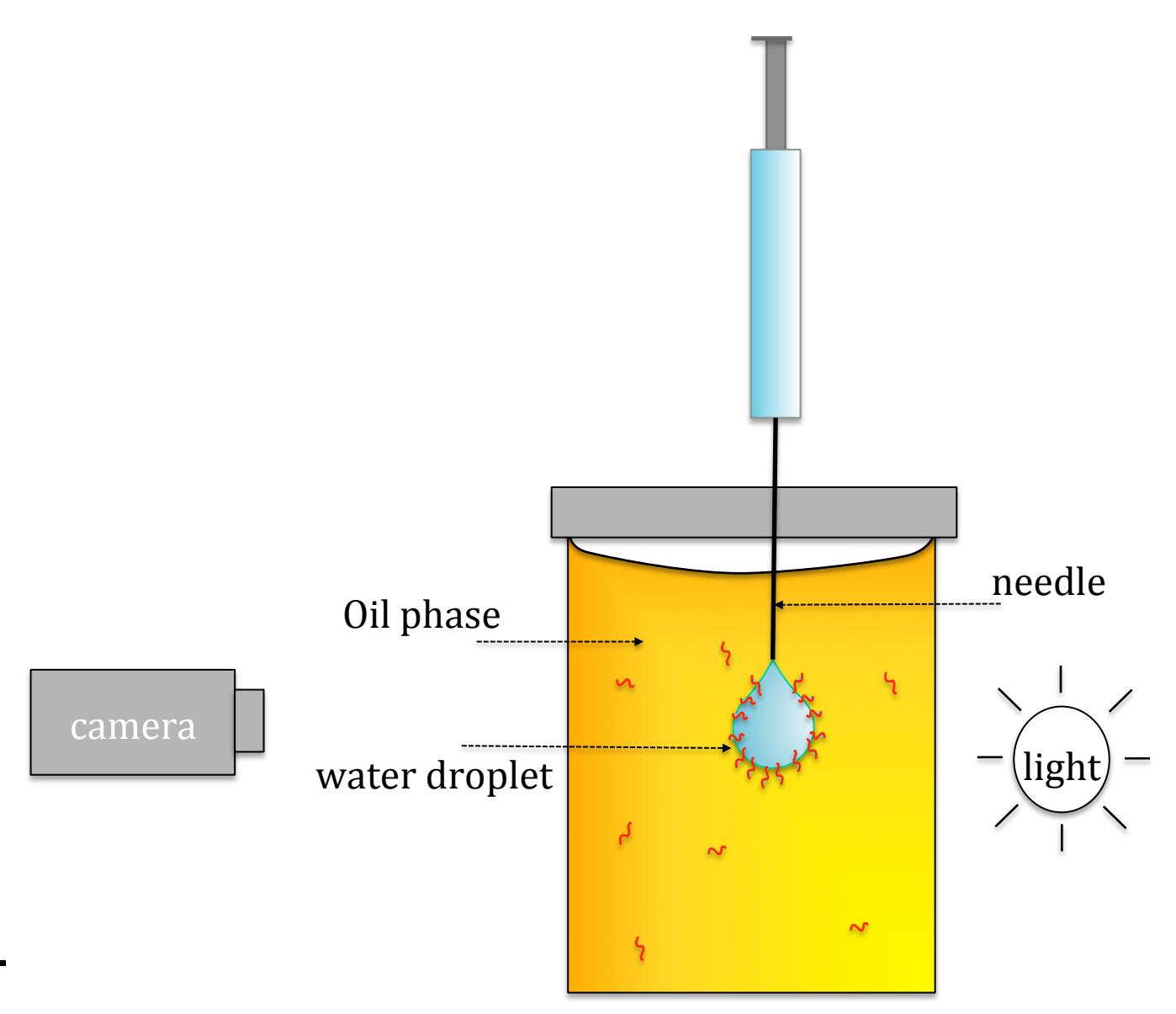
A synthetic mixture based on real products analysis was proposed containing pure compounds: trioleate and oleic acid. Interfacial tension is a key parameter for the oil droplets coalescence during the fractionation processes. The objective was to link the water-oil interfacial tensions measured with synthetic solutions to coarse-grained molecular simulation.

Characterization of lipids from microalgae & Formulation of a synthetic mixture

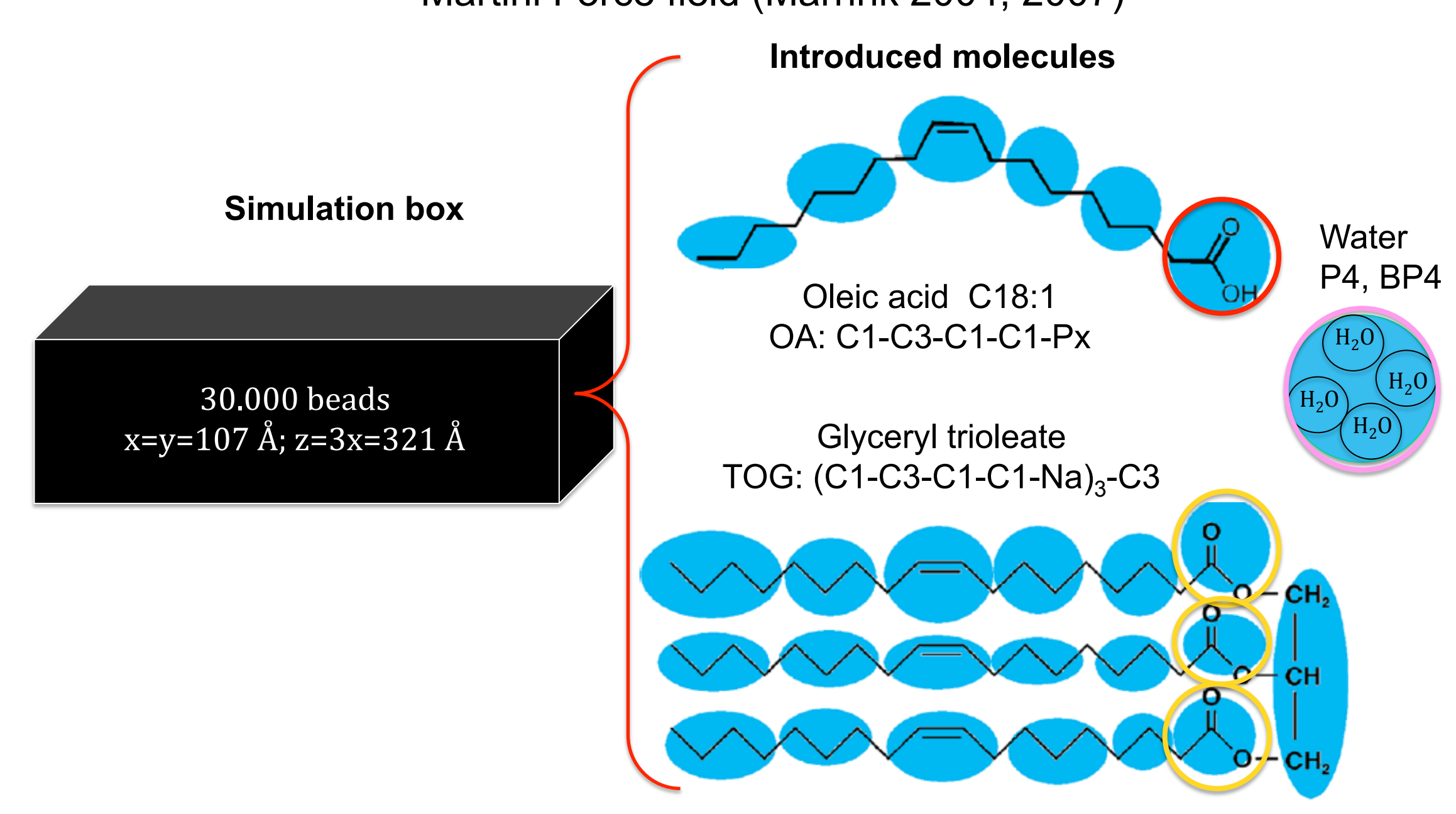


The main total fatty acids found are: oleic, linoleic, linolenic and palmitic acids.

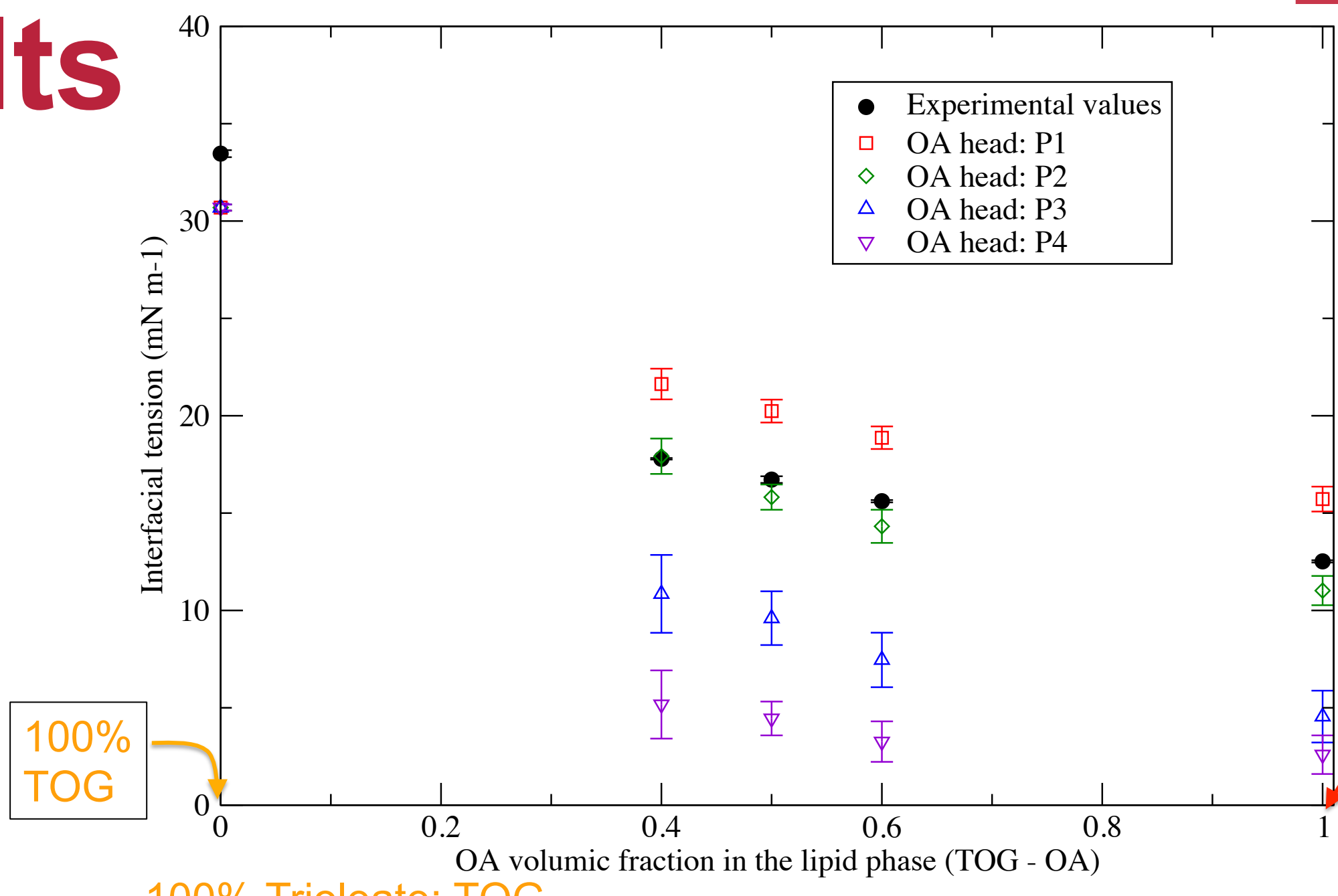
Oil-water interfacial tension measurement: γ (mN.m⁻¹)



Coarse-grained simulation of the oil-water interface



Results



The experimental values of the oil-water interfacial tension, versus TOG-OA proportion, were compared to the values extracted from coarse-grained molecular simulations. The Martini parameters described by Marrink et al. (2007) were used. Several polar particles Px are used in literature to describe the head of organic acids. We demonstrate that P2 is the best Martini parameter to describe the interfacial properties of the oleic acid.

The molecular simulation allows the understanding of the lipids organization as a function of the composition (see density figures).

In next studies we will deepen the organization of more complex mixtures containing polar lipids (phospholipids, glycolipids) and then we will introduce solid interfaces such as polymeric membranes. We will study their impact on the lipid local organization.

