INTRODUCTION

LIN (an ω-6 fatty acid) (figure 1) in water can form various structures depending on the experimental parameters. For example, it has been shown that LIN aggregate into spherical micelles at pH = 11.5 aqueous solution/medium with NaOH [1]. Micelles of LIN molecules are also used as templates to construct metal nanoparticles [2] (figure 2) and despite the widespread interest in nanosciences their structure is not well documented. We have examined by MD the micellar structure of LIN micelle solvated in explicit water with the influence of the protocol (preformed vs. self-aggregated). The aggregates obtained by the two approaches are most often similar, but sometimes they can differ. To examine this aspect, we have performed two different MD of LIN micelle with 60 molecules at ambient conditions (P = 0.1 MPa and T = 300 K).

MODELISATION OF THE LINOLEIC ACID MICELLE

The aggregation number N for the micelle simulation was obtained with a geometric model. The linoleic acid molecule displays a carboxylate headgroup that presents a surface (S_h) close to the section of the CH_2 groups (21 Å). Considering the headgroups are at the micelle surface and if the micellar hydrophobic core contains only the alkyl chains (i.e. with x=N methyl groups, with 0 < x < 17), we can write:

\[ V_m = N S_h = \frac{4}{3} \pi R_m^3 \]

\[ S_m = (1+x)N S_h = 4\pi x R_m^2 \]

Where \( L \) is the total lipid length (23 Å), \( R_m \) the micelle radius and \( N \) the aggregation number, respectively. Combining the two expressions, we obtain:

\[ 3L = (1+x)R_m^2 \]

Since the simulated micelle exhibits a significant amount of methyl groups at its surface, we can obtain the fraction of hydrophobic surface over the micelle surface:

\[ f = \frac{1}{1+x} \]

We have tested different values of \( N \) (45, 60, 75 and 90) and compared the values obtained for \( R_m \) and \( f \). Similar evolution along with the number of aggregation is found with best agreement for \( N=60 \) with an geometrical estimation of \( R_m=19.4 \text{ Å} \) and \( f=26.6\% \).

SIMULATIONS DETAILS

Two systems were constructed with two different approaches (i.e. "preformed" vs. "self-aggregated") containing 60 monomers of linoleic acid (LIN) molecule, 60 Na⁺ and 9997 TIP3 water molecules each, corresponding to a detergent concentration of 0.3 M. The preformed micelle (called M60-P) was constructed with the packmol program [4]. For the self-aggregated system (M60-S), LIN and Na⁺ were randomly placed in a water cubic box (\( a = 69 \text{ Å} \)). The resulting systems were minimized, equilibrated and subject to NPT (P = 0.1 MPa and T = 300 K) molecular dynamics simulations with full electrostatics and periodic boundary conditions using AMBER MD package [5]. We used the CHARMM27 force field for lipids with the default cis torsions parameters for the double bonds of the LIN molecule [6].

REFERENCES