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Extraction of Honduran cashew oil and interaction at the air-water interface by molecular dynamics simulation

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***Abstract*– The replacement of petroleum-derived surfactants with other environmentally correct ones such as those produced from biomass represents a window of opportunity to reduce the environmental impact of agro-industrial waste thar is currently not used, and it also represents an opportunity to promote the circular economy for the benefit of communities.**

In this work, the possibilities of using the shell of the Honduran cashew nut were evaluated, from which its oil was extracted by using a solvent, obtaining 32 – 36% oil with respect to the mass of the shell. The oil from the cashew nutshell is liquid rich in phenolic compounds such as cardanol, which, through some organic transformations, can be converted into different chemical compounds such as surfactants. To understand the structural properties of the surfactant that could be obtained from cardanol oil, the molecular dynamics technique was used, suggesting that the sizes of the tails and heads are closely related to their organization at the air-water interface, characteristics comparable to surfactants currently used in the industry, showing the viability of the substitution.

Keywords-- biorefinery, surface tension, CNSL, computer simulation

I. INTRODUCTION

Agro-industrial products and their residues can serve as the starting point for use as raw materials in a biorefinery in Honduras [1]. Its main objective is to develop new utility models in established industries by extracting chemical compounds and transforming them thereafter [2]. In this study, cashew has been taken as a reference product. Currently, in Honduras, only the fruit and the nut are used for commercialization [3]. However, the shell of the walnut is rich in phenolic compounds so they can be used as building blocks for a possible transformation through chemical reactions to products with high market value [4]–[6]. For example, it can be used in the formulation of resins, phenolics resins, polyurethanes and epoxy resins, also in the development of coatings, adhesives, emulsifiers, stabilizers and because of their antimicrobial activity they can be used in the formulation of disinfectants, bactericides and fungicides [7], [8].

Currently, the walnut shell can cause environmental problems due to its accumulation and limited utilization [9]. Presently, with the aim of guiding agribusiness to a sustainable economy, this residue has been seen as biomass for energy generation [10].

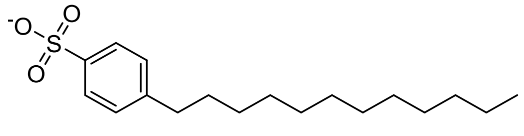
In 2014 a study was carried out in the Gulf of Fonseca, Honduras, approximately a production of 13 thousand quintals of cashew nuts per harvest was reported. From this amount, the walnut shell is not used to generate high-value products [3]. Cardanol is one of the components with the greatest versatility for post-transformation, which is present in the oil of the cashew nutshell (CNSL). Cardanol is classified as a "building block" since with the chemical transformations it can be converted into surfactants, antioxidants, fuel additives, and liquid crystals for optical materials, and fibers, among others [11], [12].

There are different recognized physicochemical methods for CNSL extraction, such as hot oil extraction, solvent extraction, mechanical extraction, vacuum distillation, and supercritical fluid bath [13]. Extraction performance varies depending on the method used. The method used in this work is the extraction of CNSL using a solvent.

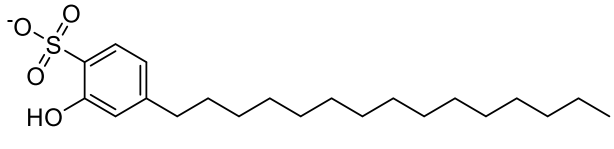
One of the transformations of cardanol is sulfonation, which produce sodium cardanol sulfonate (SCS), SCS has a structure like the linear alkylbenzene sulfonate (LABS), Figure 1. LABS is a petroleum-derived surfactant and one of the most widely used in the industry to produce detergents, emulsifiers, solubilizers, humectants, and dispersing agents. The total or partial replacement of LABS by SCS would offer a green solution to the industries [4].

LABS monolayers at the air-water interface have been extensively studied using experimental techniques and computational simulations to correlate microscopic details with macroscopic structural properties. This combination has proven successful in explaining their interaction mechanisms and making predictions about their physicochemical properties [14], [15].

Molecular dynamics (MD) simulations have proven to be a very useful tool to investigate details of the structure and dynamics of surfactants at the molecular level [16], [17]. So far, with the reviews carried out in the literature, no results have been found on the mass percentages of the extraction of CNSL in the Honduran cashew or on the molecular dynamics of SCS in the air-interface, thus this study can be served as a gateway for future research.



a) LABS



b) SCS

Figure 1. Surfactants structure a) LABS and b) SCS.

II. METHODOLOGY

A. Experimental Methodology

A batch of cashew nuts was purchased from an independent producer in Namasigüe, Choluteca. For the separation of the CNSL, reagent grade acetone with a purity of ≥ 95%, from the JT Baker brand was used, meeting the chemical requirements of the ACS. Distilled water from the Labhospy brand was used, with a conductivity of 18 MΩ-cm as reported by the manufacturer.

For the pretreatment, the nuts were classified and washed using a mixture of water and commercial detergent [18]. Once cleaned, they were place in a container with a 3% sodium hypochlorite solution, and they remained in contact for 18 h [19]. They were sun-dried, and after that, the shell was separated from the nut using equipment specifically designed for this purpose. The apparatus used enables controlled and efficient separation applying pression, minimizing damage and ensuring the integrity of the shell. On a laboratory scale, the shells were crushed using a disc mill, obtaining a particulate material between 5-15 mm. The crushed material was stored in a cool, and dry place [18].

A 1000 mL of a 45/40 Soxhlet extractor was used for the extraction process [20]. The experimental setup included a round-bottom flask, a reflux extractor, a bubble condenser, a Lab Companion HP-3100 series heating plate with a temperature range from 0 to 380 °C, and a distillation unit for separating the oil. In a round-bottom flask 300 mL of acetone were added. 50 g of the crushed shell were weighed and placed inside a Soxhlet 40/45 thimble made of grade 603 cellulose with a diameter of 30 mm, which was put in the Soxhlet extractor. All the parts of the apparatus were assembled, including the flask containing the acetone. Acetone was heated under reflux to maintain a constant volume. This process continued until no further changes in the color of the solvent were observed, which took about 2.5 to 3 h. The oil and solvent, known as extraction crude, while still hot, was transferred to an amber bottle for subsequent separation through a distillation process. The simple distillation setup of Corning brand and Pyrex 24/40 material included a three-neck flask, cold finger condenser and collecting flask, with their adapters. The crude extract was added to the distillation flask, and heating was initiated, approximately 2 h, to evaporate the solvent and obtain the CNSL.

B. Simulation Methodology (MD)

To carry out the simulation, GROMACS, version 2018 computational package used was [21] [22]. CHARMM27 atomistic force field [23] was used for all simulated models. The LABS and SCS structures were created using the molview program, generating a file with the structure in mol format which was changed to mol2 using the openbabel program [24]. The enhanced structures and parameterization of LABS and SCS were generated using SwissParam [25]. The charges and force constants of the hydrophilic LABS head were taken from *He et al.*[15]. On the other hand, only the SCS head loads were manually assigned based on the LABS model, the rest of the parameters were kept the same as those of CHARMM27. The SPC/E model of water was used for water molecules [26]. Periodic boundary conditions were applied in all directions along the Cartesian XYZ axes. Newton's equation was solved using the Leag-frog algorithm [27] with an integration time of 2 fs. For nonbonding van der Waals and Coulomb interactions, the cutoff radius was 1.2 nm. A cutoff radius of 1.2 nm was used for long-range nonbonding interactions with the Edwal particle approach. [28]. With the LINCS algorithm all bonds were restricted [29]. The isothermal compressibility constant used was $4.5x10^{-5}$ bar^{-1}.

The LABS and SCS monolayers, each containing 144 molecules, were constructed using the PACKMOL script [30]. The gmx editconf program was used to create a 9.3x9.3x15 nm box, the symmetrical monolayers were arranged, with the heads of the surfactants facing each other at 5 nm. A water box was created with the same XY dimensions as the monolayer-monolayer system but with a height of 5 nm, using the gmx solvate program. The box contained approximately 5500 to 14000 water molecules. Using the gmx editconf program, the coordinates of the monolayer-monolayer system and the water box were merged into a single system. To neutralize the system, 288 water molecules were replaced with 288 sodium ions.

Energy minimization was performed to equilibrate both systems using the steepest descent algorithm, with a maximum force threshold of 1,000 kJ mol^{-1} nm^{-1}. Two equilibration stages were carried out before the molecular dynamics simulation. In the first stage, the temperature was equilibrated at 298 K for 1 ns with the v-rescale thermostat [31], and with a coupling time of 0.1 ps by NVT ensemble. In the second stage, the NPT ensemble was used with the Raham Parrinello barostat [32] to equilibrate pressure to 1 bar with a coupling time of 5.0 ps for 1 ns. Using the Nosé Hoover thermostat, molecular dynamics were performed with an NPT ensemble and leadfrog algorithm for 1 microsecond for LABS and 0.5 microseconds for SCS [33]. A coupling time of 0.5 ps to control the temperature at 298 K and barostat Raham Parrinello [32] with a coupling time of 2.0 ps and 1 bar of pressure. All analysis were performed with the last two 200 ns of molecular dynamics. An Outline of the simulation stages followed by MD simulation are showed in the Figure 2.

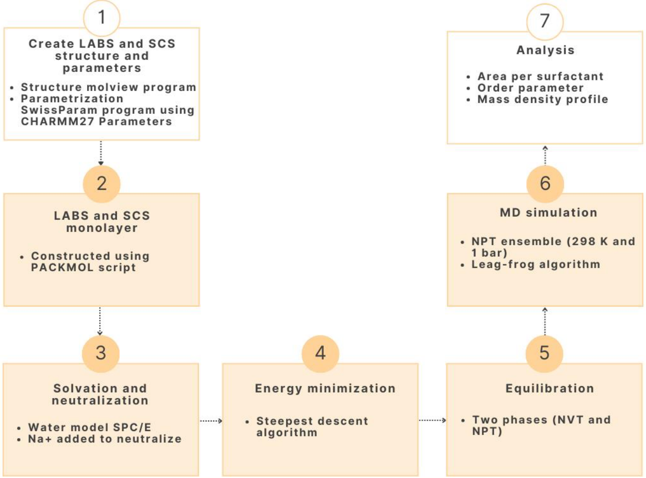
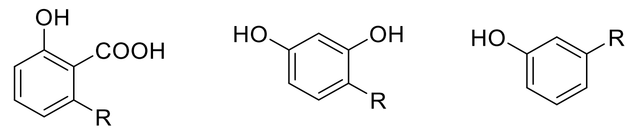


Figure 2. Outline of the simulation stages followed by MD simulation.

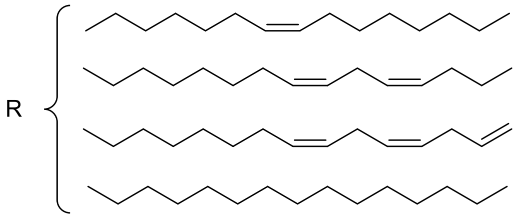
II. RESULTS AND DISCUSSION

A. *Extraction CNSL*

CNSL extraction was performed using acetone, a polar aprotic solvent. Various solvents, such as acetone, hexane, methanol, toluene, and petroleum ether, have been evaluated for the extraction of CNSL. Comparative results indicate that acetone yields a CNSL extract with properties that closely match those of the used in industrial applications [18][20]. It is anticipated that aprotic polar solvents will not significantly affect the physicochemical properties of the oil, as they are not hydrogen bond donors and therefore cannot induce dimerization with the phenolic compounds in the oil. Furthermore, these solvents provide effective solvation due to the intermolecular interactions they exhibit with the CNSL compounds. CNSL is a mixture of anacardic acid (2-hydroxy-6-pentadecylbenzoic acid), cardol (5-pentadecylresorcinol), and cardanol (3-pentadecylphenol). These compounds have hydrocarbon chains of 15 carbons, which vary according to their unsaturation (mono-, di- and tri-ene) as shown in Figure 3.



a) Anacardic acid b) Cardol c) Cardanol



d) Hydrocarbon chains of 15 carbons

Figure 3. Structures of the main phenolic components in CNSL.

Note. Description of each structure: a) anacardic acid, b) cardol, c) cardanol and d) hydrocarbon chains of 15 carbons.

Several extractions were performed with acetone for subsequent removal through distillation, obtaining a deep dark brown oil, Figure 4. The amount obtained from this oil represents between 16–18% of the total mass of the pretreated nut, results comparable to those reported by Balachandran and collaborators who describe a recovery range between 18–25% [4]. The lower values obtained in the present work may be attributed to the process used to reduce the particle size of the shell, as some material is retained on the mill disc. Recovery could be enhanced by using liquid nitrogen during the milling process [13].

Considering only the mass of the crushed shell that comes out of the mill, the extraction percentage was 32–36%, values higher than those reported by Garkal and Bhande, who obtained values of 25–30%.[34]. These results suggest a distinct difference between walnuts from Honduras and those from other producing countries. Countries such as India and Brazil have a higher yield of the nut fruit compared to Honduras, indicating that the varieties produced in Honduras have a greater shell mass, likely due to the genetic variability of the nuts [3].

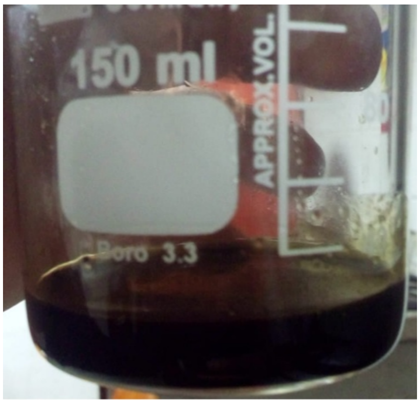


Figure 4. Picture of CNSL after removal of extraction solvent

B. *LABS and SCS molecular dynamics*

Three analyses were performed to elucidate the structural information of LABS and SCS monolayers. The analysis discussed included area per surfactant, order parameter, and density profile. The area per surfactant is a measure used to show stability over time of the interface, as well as organization. The order parameter is a measure of spatial orientation, for this study, the carbon atoms of the LABS and SCS tails were analysed along the axis perpendicular to the air-water interface (Z). The order parameter can range from 1 (completely ordered along the Z axis) to -0.5 (completely ordered along the axis perpendicular to the Z axis). The density profile also provides the orientation of specific atoms or groups in the system.

Figures 5 and 6 show the LABS and SCS systems in their initial and final configuration, both systems show stability before 100 ns of dynamics. The results of the XY area of square angstrom per surfactant for the LABS and SCS are observed in Figure 7. On the one hand, the LABS shows an average area of 26.3 ± 0.3 Å^2. On the other hand, the SCS shows a smaller average area of 21.7 ± 0.2 Å^2. The area average value of the SCS is close to the experimental and theoretical value of stearic acid, 20-22 Å^2 reported by Griffith [35]. Stearic acid has a 17-carbon hydrocarbon tail. In another study, a molecule with the same tail length as stearic acid but with a modification to its head exhibited an area similar to that of stearic acid, 21.5 Å^2 [16]. These results indicate that the length of the surfactants tail may play a crucial role in calculating their area per surfactant. The SCS system presents a greater packing, this could be the result of the changes in its structure concerning LABS: a head with the addition of the hydroxyl group, probably a greater formation in the number of hydrogen bonds with water, and with the other heads and a longer hydrocarbon chain, 15 carbons.

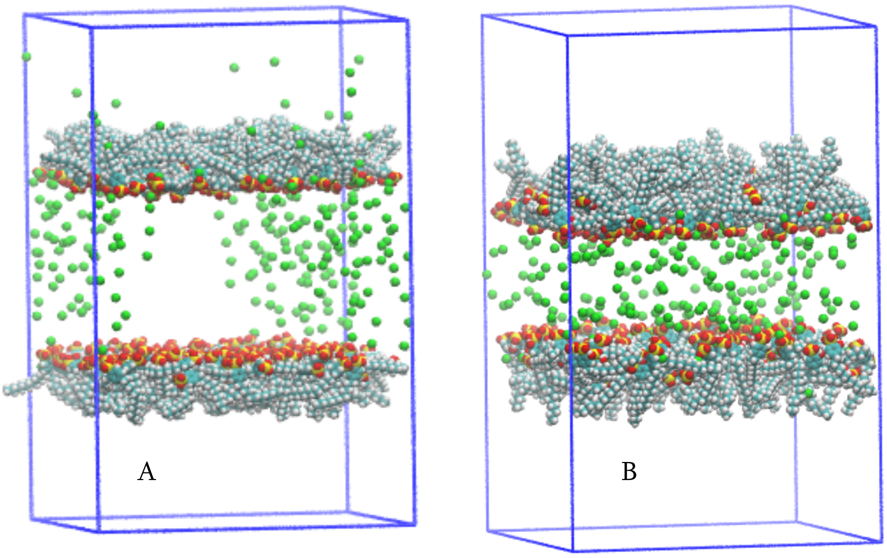


Figure 5. Initial system configuration LABS (A) and SCS (B).
Note. Systems LABS (A) and SCS (B) before equilibrium, initial configuration. Water molecules are not presented in the snapshot to give visibility to sodium ions (green), hydrocarbon chain (white and turquoise) and head (yellow and red).

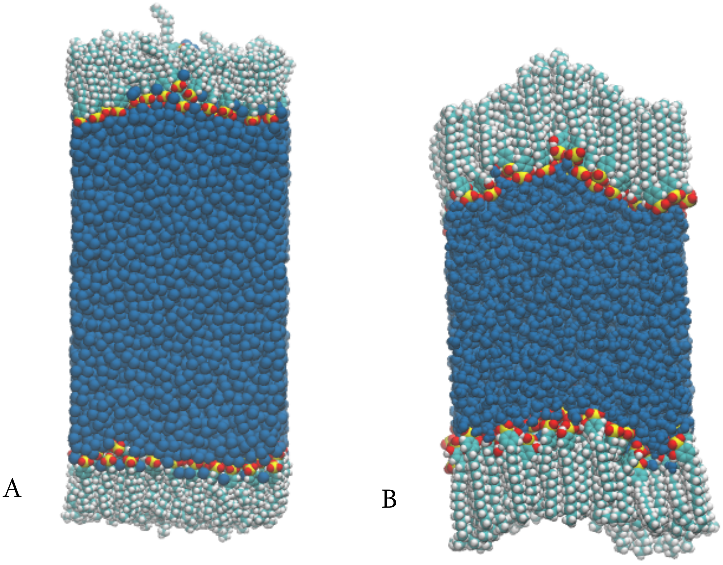


Figure 6. Final system configuration LABS (A) and SCS (B).
Nota. System LABS (A) and SCS (B) after 1,000 ns y 500 ns, respectively. Hydrocarbon chain (white and turquoise), head (yellow and red) and water (blue).

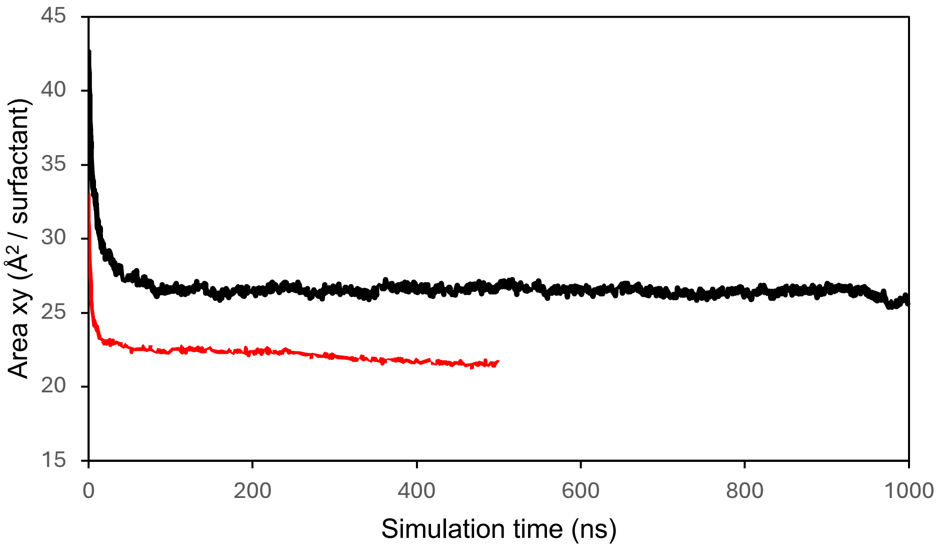


Figure 7. Area per surfactant of LABS and SCS.
Note. Area per surfactant in Å^2 of LABS (black) and SCS (red) for 1,000 ns y 500 ns, respectively.

This greater packing is also evident in the calculation of the order parameter, Figure 8. SCS shows greater organization than LABS. Evidence suggests that increasing the number of carbons in the surfactant tail, 12 to 15, enhances the organization of the carbons farthest from the head. The improved organization resulting from an increase in the number of carbon atoms in the surfactant tail is furthered demonstrated by [16], the surfactant under analysis with a 17 carbons tail shows an S_{CH} between 0.3 and 0.45 while the SCS between 0.3 and 0.4. In this same study, a behavior like that of the SCS can be observed, with comparable values for nearly all the carbons in the tail center. A breaking point in the behavior of the carbon atoms can be observed from carbon 9. In LABS, a significant decrease in its organization is observe in the terminal carbons. However, this decrease is more gradual in the terminal carbons of the SCS. This distinction could be attributed to the increase in intermolecular forces that overcome when having a longer hydrocarbon chain.

A density profile of the various functional groups comprising the surfactants can provide insight into their position within the system. Figure 9 shows the density profiles for the groups: water, head, and hydrocarbon tail of LABS and SCS, the profile displays a symmetrical behavior as expected by the original design of the monolayers. Both systems exhibit a water layer density very close to 1,000 kg m^{-3}, a result that corresponds with its experimental value. A difference in the water layer width is evident between LABS and SCS, due to the different amount of water added each system. The SCS system shows a greater integration of the head and tail groups into the water layer. A more thorough analysis of the surfactants head groups shows the electrostatic charge distribution, characteristic of ionic surfactants. The electrostatic repulsion generated between micelles in the detergency phenomenon is responsible for the stabilization of the systems and prevents their coalescence. Figure 10 shows that both systems exhibit an electrical double layer formed between a sulfonated negative head and its positive sodium counterions. Like the general density distribution, it is observed that, in the case of SCS its different groups are more immersed in the water layer. In both cases the sodium ion is completely immersed and aligned at the interface. Noting that, although the sodium ions were randomly distributed within the water layer (Figure 5), they migrate to the interface to stabilize the monolayer.

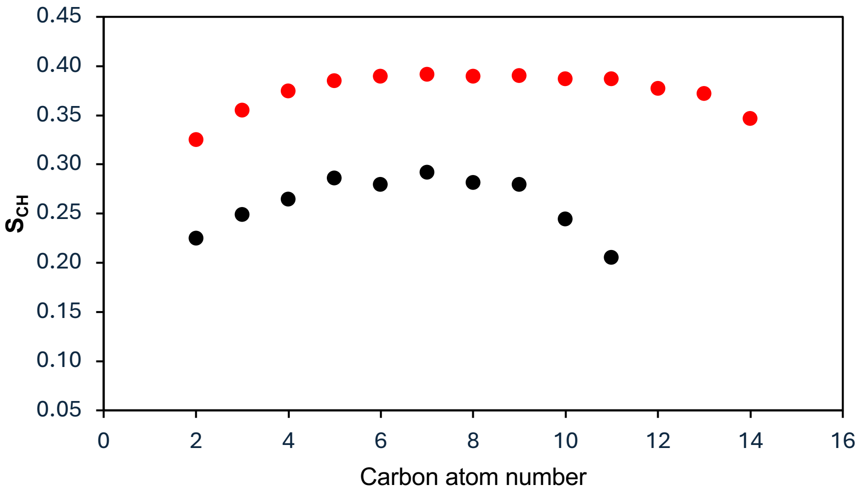


Figure 8. Orden parameter of tail carbon atoms of LABS (black) y SCS (red)

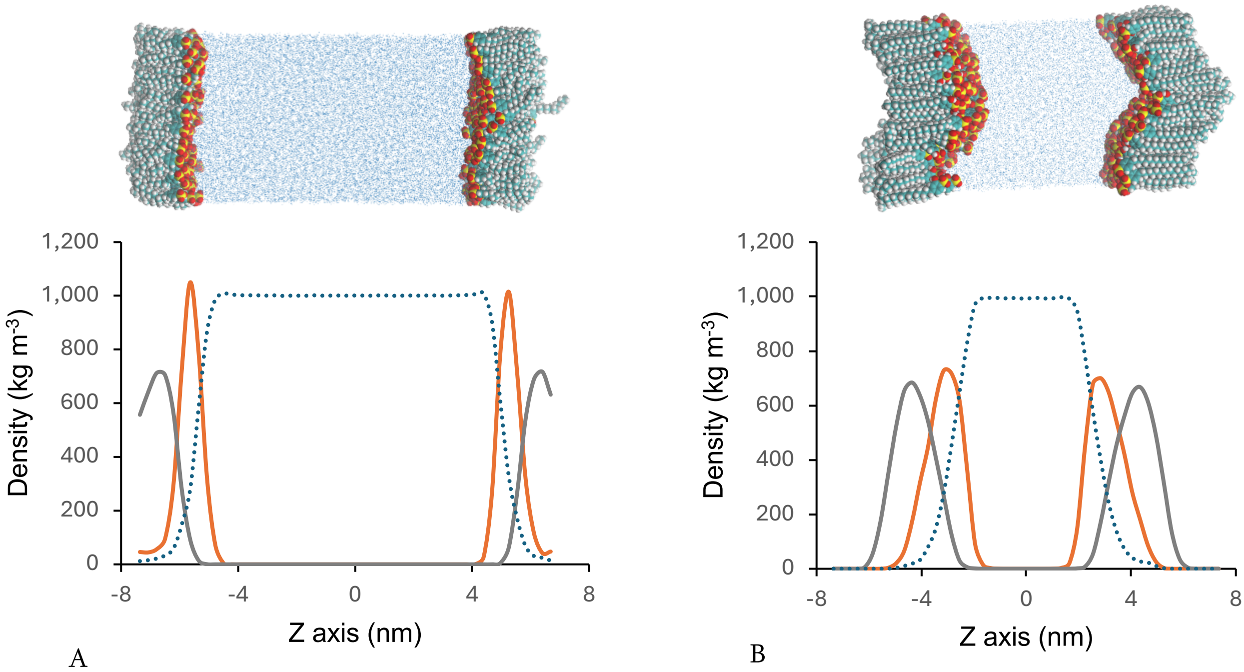


Figure 9. Mass density profile LABS (A) and SCS (B).
Note. Mass density profile (kg m^{-3}) along the Z axis (nm) of water (blue), head (orange) and hydrocarbon tail (gray) of the systems with the surfactants de LABS (A) and SCS (B).

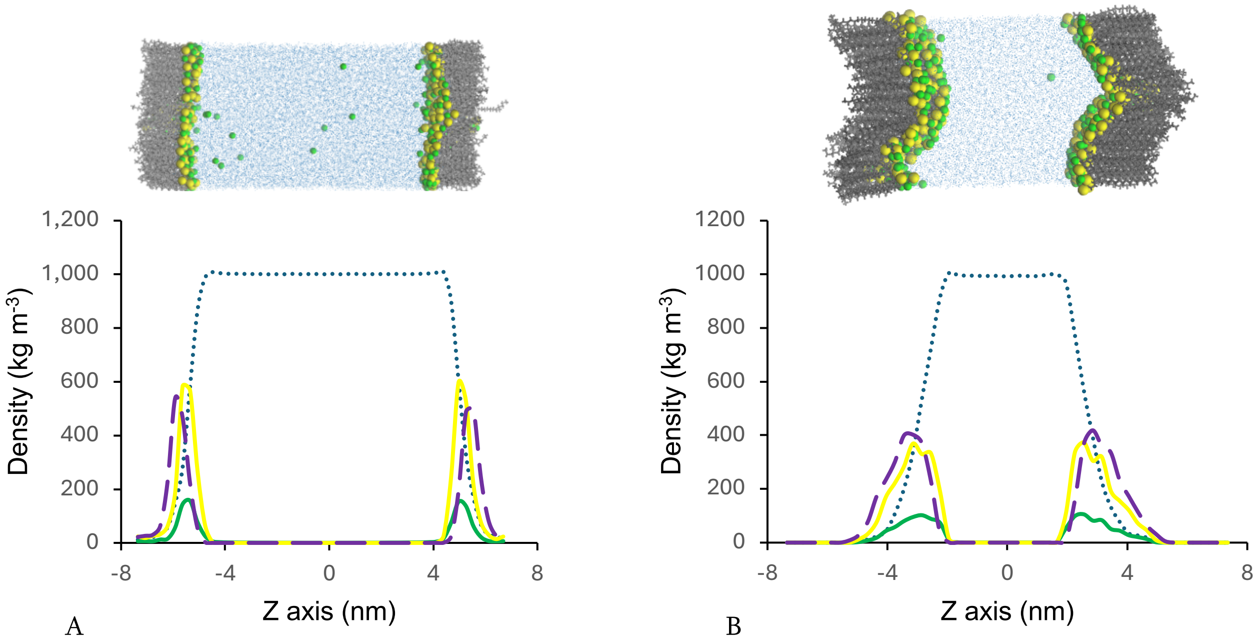


Figure 10. Mass density profile LABS (A) and SCS (B).
Note. Mass density profile (kg m^{-3}) along the Z axis (nm) of water (blue), SO_3^{-1} (yellow), benzene (purple) y Na^+ (green) of system with surfactants LABS (A) and SCS.

III. CONCLUSIONS

The CNSL extraction was performed using a Soxhlet type extractor. The experimental results indicate that the shell of the Honduran cashew, Anacardium occidentale, contains noteworthy percentages of CNSL, comparable to or even exceeding those reported for varieties cultivated in countries such as India and Brazil. These preliminary findings underscore the importance of promoting research and technological development aimed at the integral utilization of this by-product, which has traditionally been considered waste. Its valorization would not only contribute to reducing agro-industrial waste but also add value within the local production chain, positioning Honduran cashew as a strategic source of bio-based inputs within the framework of a circular and sustainable economy.

LABS and SCS molecular dynamics of 1 and 0.5 microsecond simulations were successfully performed using the GROMACS 2018 computational package and the CHARMM27 atomistic force field. Results for area per surfactant, order parameter and density profile indicate that the SCS monolayer remains stable over time, a conclusion that was also confirmed for LABS. Structural analysis demonstrates the impact of head and tail sizes on surfactants: a larger hydrocarbon tail leads to greater organization, while a hydrophilic head enhances solvation at the interface.

The oil extraction and successful computational simulations presented in the study open a window of opportunity for further research, leading to the extraction of cardanol and its chemical conversion into other compound of interest with significant industrial applications.

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