Study of competitive adsorption of heavy metals in SDS and rhamnolipid micelles by molecular dynamics

Ana Beatriz Salazar Arriaga
Facultad de Química
Universidad Nacional Autónoma de México
email: betyann775@hotmail.com

Heavy metal contamination of water bodies represents a major environmental problem, which has driven the search for more efficient and sustainable remediation methods. Among the proposed strategies, the use of micellar systems for the capture of these pollutants has attracted growing interest. However, the molecular mechanisms governing the competitive adsorption of different metal ions are not fully understood. In this work, molecular dynamics simulations were used to investigate the adsorption affinity of various heavy metals in two micellar systems: the synthetic surfactant sodium dodecyl sulfate (SDS) and the rhamnolipid biosurfactant. The analysis of simulation trajectories, radial distribution functions, and density profiles allowed for the characterisation of the interaction between the ions and the polar groups of the micelles. The results show that divalent cations have a higher affinity for polar groups; in particular, ions such as Zn^{2+} and Ni^{2+} exhibit the most favourable interactions with both micellar systems. Furthermore, it was observed that SDS micelles present a higher metal retention capacity than rhamnolipid micelles, evidencing important differences in the adsorption mechanisms between a synthetic surfactant and a biosurfactant. These findings provide molecular level information on the competitive adsorption of heavy metals and contribute to the design of more efficient and sustainable surfactant-based environmental remediation systems.

Ana Beatriz Salazar Arriaga earned her Bachelor's degree in Chemical Engineering from the National Autonomous University of Mexico (UNAM). She received both her M.Sc. and Ph.D. degrees in Materials Science and Engineering from UNAM, graduating with honors in both programs.

Her research focuses on molecular simulation and modeling of complex systems, with particular emphasis on the physicochemical properties of interfaces. Her work is centered on the study of surfactants and biosurfactants, with applications in environmental remediation and the design of functional materials. She has authored 13 peer-reviewed scientific publications in international journals. Salazar Arriaga has extensive teaching experience at UNAM, where she has taught undergraduate and graduate courses, including Molecular Simulation: Theory and Applications, Contemporary Physics, and Thermodynamics. She was awarded the Alfonso Caso Medal for outstanding academic achievement during her master's studies and received the BAL-UNAM Earth Sciences Award in 2022. In addition, she was recognized for one of the best poster presentations at the 13th Meeting on Molecular Simulation in 2023. She is also actively involved in science outreach through conference presentations, public engagement activities, and the development of educational audiovisual content for digital platforms.