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A Computational Study on the effects of Temperature and Osmotic Pressure on Water Extraction on Microalgae using Big Multipole Water – Martini Forcefield on GROMACS Simulation

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Abstract: Microalgae as a biofuel has been the interest of researchers because it is one of the sources of renewable biodiesel that is capable of meeting the global demand for transport fuel without competition on human food consumption. Drying the microalgae down to ten percent (10%) of its weight in large scale production that is cost and energy efficient has been the challenge for researchers in order to fully utilize its oil content and without producing soap. In this study, GROningen MAchine for Chemical Simulations (GROMACS) is utilized to provide a theoretical explanation on the mechanism of water extraction from the microalgae using the latest Big Multipole Water (BMW) – MARTINI Coarse-grained forcefield which gives more fundamental membrane properties and improved energetics when compared to the original MARTINI forcefield for the interactions at the membrane-water interface. To represent the *Chlorella Vulgaris* microalgae in molecular dynamics, Dioleoyl-sn-glycero-3-phosphocholine (DOPC) was used which is the dominant lipid in a microalgae excluding membrane proteins. In this study, the temperature was varied from 300 K to 410 K with 10 K increment to verify the effects of temperature on the thickness and layer structure of the DOPC which provided a deeper explanation on the traditional method of drying by introducing thermal energy. Moreover, a minimum osmotic pressure of 150 MPa was determined that exhibits extraction of water from the microalgae by applying acceleration on water in our simulation on non-walled periodic system.

Key Words: Microalgae; GROMACS; DOPC; Osmotic pressure; BMW- Martini