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Molecular Structure and Formation of Melatonin in the Bulk Water and at the Water–Air Interface: A Molecular Dynamics Simulation Study

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Melatonin (N–acetyl–5–methoxytryptamine) is a natural hormone produced by the pineal gland, located behind the third ventricle in the brain that it is used to control the human sleep cycle. Consequently, it has been widely used as a drug for the treatment of the sleep disorder. Melatonin encapsulated niosome particle is an important key for drug delivery application. It is well–known that the melatonin has hydrophilic and lipophilic properties which enable it to pass easily into any cell, fluid or compartment within the body. In this study we report the molecular structure and dynamical properties of the melatonin molecules in the bulk water and at the water-air interface. Molecular dynamics simulations were performed at the temperature of 298 K and the pressure of 1 bar was simulated until it reaches to equilibrium. Afterward the structural and dynamical properties of the melatonin which are randomly distributed in the bulk water and at the water–air interfaces were calculated and compared with the previous studies. In the case of the melatonin in the bulk water, the simulation indicates that the melatonin molecules favor to form aggregation by separated from the bulk water, which is quite obvious. This implies that the melatonin exhibits more solubility in lipid phase than the water phase. In the case of the melatonin randomly distributed on the water–air interface, the simulation reveals that the melatonin molecules favor to form the monolayer film at the interface. The melatonin tailgroups favor to adsorb on the water surface while their headgroups point to the air phase. For the two systems, the self–diffusion coefficient of the water was calculated, and finding it decreasing ˜ 36.1 % from the pure water simulation. Such characteristics shows that the self–diffusion coefficient of the water is reduced due to obstruction effects in which are similarities to that reported for surfactant self–assembly formation in solvent. In addition, we also find that the probability for hydrogen bond formation between the melatonin–water molecules of the two systems are occurred as follows: Carbonyl Oxygen(acceptors)–HW(donors), Indole NH(donors)–OW(acceptors), Amide NH(donors)–OW(acceptors), and Methoxy Oxygen(acceptors)–HW(donors), respectively. While, the melatonin–melatonin molecules of the two systems are occurred as follows: Indole NH(donors)–Carbonyl Oxygen(acceptors), Amide NH(donors)–Carbonyl Oxygen(acceptors), Indole NH(donors)–Methoxy Oxygen(acceptors), and Amide NH(donors)–Methoxy Oxygen(acceptors), respectively. Fortunately, this model can be good reproduced the quantum chemistry calculation that reported previously for the hydrogen bond formation.

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