Waraporn Boonyarat 2010: Molecular Dynamics Simulations of Vitamin E and Inulin in the Lipid Bilayer. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Miss Patchreenart Saparpakorn, Ph.D. 79 pages.

Currently, the uses of foods which may exert a positive functional effect on health are widely focused. Two of these functional foods are known as probiotics and prebiotics, which have a favourable effect on the good bacteria that reside in digestive systems, also known as gut micro flora. Probiotics actions are the synthesis of short-chain fatty acids (SCFAs) and vitamins. In addition, prebiotics are natural saccharides that locate the large intestine undigested. Difference between probiotics and prebiotics is absorbed into intestina. This absorption of probiotics and prebiotics is unclear and interesting to study the mechanism. In this study, the distribution of Vitamin E (probiotic) and inulin (prebiotic) at water/membrane interface has been investigated by molecular dynamics (MD) simulations. The MD simulations running on the time of 10 ns were carried out in the same conditions by using GROMACS software and the SPC (single-point charge) parameters were used. The dipalmitoylphosphatidylcholine (DPPC) bilayer was stabilized by the energy minimization at 323 K and 1 bar as constant**.** The MD study focused on favorable binding sites of Vitamin E and inulin embedded into DPPC bilayer. The simulations were shown that vitamin E was preferably accommodated at the head of the bilayer upper the glycerol moiety. In addition, it was found that the hydrophobic aromatic part of the vitamin E was located inside more ordered region of DPPC from the hydrophobic character of vitamin E. The snapshots revealed the depth of the vitamin E localization which was gradually shifted deeper inside the hydrocarbon core of the bilayer. The results showed that the vitamin E showed weak hydrogen bonding to DPPC bilayer and the distribution of vitamin E molecule simulations was presented at the opposite of the entrance. The depth of the inulin localization was shifted deeper inside between the phosphate and glycerol core of the bilayer. Moreover, the possibility of the penetration of the inulin through the bilayer was analyzed. During our MD analysis, we found that cannot cross the bilayer from one leaflet to the other. The strong hydrogen bond was found between hydroxyl group (OH) of inulin and oxygen atoms of phosphate and glycerol.

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