

26 – 29 May 2013, Kyiv, Ukraine

Using molecular dynamics for study butter

Sergii Ivanov, Tamara Rashevskaya, Victorya Shapoval

National University of Food Technologies, 68 Vladimirskaya St., Kiev, Ukraine, 01601
rashevsk@nuft.edu.ua

ABSTRACT

Atoms are elements that creating are all materials in our world: stone, wood, salt and of course dairy butter. Scientists of our university have been studing nanostructure of butter for a long period. In particular, the functional food supplements impact on quality and nanostructure of butter. For better understanding process taking place in butter we began to study butter structure at atomic level. Large number of structure components makes it very difficult to research. We need a computer help. We have used molecular dynamic method, program ChemBioOffice2012 in particular. These methods are now routinely used to investigate the structure, dynamics and thermodynamics of biological molecules and their complexes. According to the research of our university it is well-known that inulin addition in butter formes strong inulin-lipid membranes of shell on milk fat globules. We trying to study what inner processes are working. With the help of program ChemBioUltra3D, the process of interaction between inulin polysaccharide and phosphatidylcholine (a type of phospholipid in lecithin) has been simulated. Lecithin is one of the components of protein- phospholipid membrane of milk fat globules. Molecular structure of inulin and phosphatidylcholine were taken from international Protein Data Bank. PDB is a source of proteins and nucleic acid 3-D structure, well-known among scientist all over the world. And we have used information from biochemistry books. We have received the 3-D model and tracked changes in the spatial structure of the compound in a time interval of 10 fs. This method can be used to study the properties of butter with vegetable food additives at the atomic level.

KEY WORDS

Butter, inulin, lecithine, molecular dynamics, phosphatidylcholine.

Indicate type of presentation: **Poster**