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# Molecular Dynamics and Monte–Carlo Simulations for Replacement Sugars in Insulin Resistance, Obesity, LDL Cholesterol, Triglycerides, Metabolic Syndrome, Type 2 Diabetes and Cardiovascular Disease: A Glycobiological Study

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## Editorial

Ketonic monosaccharide and disaccharide sucrose have long been added to Fructose, Glucose and Galactose to improve their biochemical, glycobiological and biological properties [1–11]. Ketonic monosaccharide and disaccharide have begun to replace larger sugars in insulin resistance, obesity, LDL cholesterol, triglycerides, metabolic syndrome, type 2 diabetes and cardiovascular disease because they can impart different properties such as biochemical, glycobiological and biological properties, at the same time, provide property enhancements at lower loadings sugars form a variety of ordered structures on nanometer length scales, allowing them to severe as a ordered matrix for Fructose, Glucose and Galactose which add functionality to the sugars [11–21]. Discontinuous molecular dynamics simulation is used to study the phase behavior of Fructose, Glucose and Galactose [22–25]. Considerable effort has been devoted to theoretical and computational simulation studies of sugars phase behavior [26–31]. This editorial describes the models used for phase diagrams of self–assembled mono–tethered nanospheres (TNS) from molecular simulation and comparison to larger sugars. An impressive variety of Fructose, Glucose and Galactose of different sugars and geometries has been synthesized. Also, in this editorial, we aim to predict the assembled structures formed from Fructose, Glucose and Galactose as well as to compare with larger sugars. Moreover, we have developed a model for self–assembled mono–tethered nanospheres (TNS) and perform Brownian Dynamics (BD) simulations to investigate the tendency for these model self–assemble.

On the other hand, this editorial is in the use of quantum chemical methods for phase equilibrium. We focus on two computational methods related to thermodynamic and biospectroscopic properties and phase behavior. The first is a conceptually straightforward application in which one uses interaction energies between High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules obtained from quantum chemistry in Monte–Carlo simulation to compute High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules thermodynamic and biospectroscopic properties. This has been done as a two–step process. First, the interactions between High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules are computed from *ab initio* quantum chemistry. These energies are fit with a model potential function and then used in simulation. Then, in the second step, *ab initio* calculations have been used to compute interaction energies between High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules. These energies are then used as the interaction energy parameters in the widely used Wilson and UNIversal QUAsiChemical (UNIQUAC) activity coefficient models. Excellent predictions are obtained with the UNIversal QUAsiChemical (UNIQUAC) model, whereas poor results are found with the Wilson model. In addition, using the same parameters and the UNIversal QUAsiChemical (UNIQUAC) model, high–pressure vapor–liquid equilibriums predictions were made. The low– and high–pressure results demonstrate that this unique approach can lead to accurate vapor–liquid equilibrium prediction for Hydrogen–bonding mixtures in High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules.

Furthermore, Monte–Carlo simulation of a three–dimensional (3D) lattice model of the amphiliphiles–solvent systems are presented and examined for their usefulness in predicting the thermodynamic of self–association of amphiliphiles in High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules. Thermodynamic and biospectroscopic parameters are studied by lattice Monte–Carlo simulation including aggregation number and critical High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules concentration. The regular excluded volume and periodic boundary conditions are used to mimic a box of simulation as High–Fructose Corn Syrup (HFCS) (Glucose–Fructose, Isoglucose and Glucose–Fructose syrup) molecules.

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