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Forecasting The Molecular Properties Of Dietary Supplement Used In The Recipe Of Foodstuff For Diabetes Mellitus Prevention.

Vladimir Vsevolodovich Sadovoy[1,2]*, Tatiana Viktorovna Shchedrina[1], Veronika Valerievna Melentyeva[2], and Alla Smalievna Khamitsaeva[3].

[1]North-Caucasian Federal University, Ukrainskay St., 56 "A", 357500, Pyatigorsk, Russia.
[2]Stavropol Institute of Cooperatives (branch) BUKEP, Goleneva St., 36, 355006, Stavropol, Russia.
[3]Gorsky State Agrarian University, Kirov St., 37, 362040, Republic of North Ossetia-Alania, Vladikavkaz, Russia.

ABSTRACT

When analyzing diets of people with diabetes mellitus, a deficiency of lecithin, vitamins B1 and PP was revealed. Using Langevin dynamics, the molecular properties of the investigated biologically active additives in the initial conditions and in the process of heat treatment are studied. It has been established that the molecules of lecithin, vitamins B1 and PP do not become excited during the heat treatment as part of the meat product formulation and retain their original properties, which is also indicated by their quantitative content in the finished product. As a result (by the example of a composition in a meat food that was subjected to heat treatment), it has been confirmed that lecithin, vitamins B1 and PP can be used in foodstuff formulas for people with diabetes mellitus.

Keywords: molecular organization, geometric optimization, molecular properties, thermal conditioning.

Corresponding author

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INTRODUCTION

Diabetes mellitus is rightly called the "non-infectious epidemic of the 21st century". The number of people with diabetes mellitus among the various population groups in the world doubles every 13 to 15 years. The fight against this disease is currently one of the important health problems of highly developed and emerging countries. When assessing the availability of diabetic patients with main essential components, it was found that in most cases the usual diet does not compensate the increased body needs for these vital substances [1, 2]. On the basis of the performed analysis, a special deficiency of B1 vitamins (0.42-0.55 mg / day), PP (4.46 - 5.26 mg / day) and lecithin (4-5 g / day) was noted. Taking into account the norm of animal protein consumption, it is established that vitamins B1 in the amount of 0.21 - 0.28 and PP - 1.73 - 2.13 mg per 100 g of product must be introduced into the designing antidiabetic composition [1].

One of the remarkable discoveries was the discovery of the physiological properties of the dietary supplement lecithin. It helps to reduce insulin requirements for diabetics, if a diabetic patient regular intakes lecithin, it protects the liver from steatosis. Lecithin is simultaneously the main component of the cellular membranes of the whole organism, the most important fat emulsifier, an effective cholesterol carrier and dissolver. It is able to stabilize the bile and restore cells of the liver and lungs, participates in neurotransmission (transmission of the nerve impulse) and the functioning of brain tissue actively. At the same time it is the source of such important vitamins as a choline, as well as a number of non-esterified fatty acids that are necessary for work of the hormone system. Studies have shown that the body of a healthy person synthesizes only one-fourth of the required lecithin. The rest 3/4th should come with food. According to the nutritionists' recommendations a modern healthy person needs at least 5-6 grams of lecithin daily. The internal organs, receiving less than the necessary for their living expenses, begin to be overloaded. This leads to increased "wear and tear" of the body, poor health and reduction of the overall health [2].

Vitamins also take an active part in the metabolic control of carbohydrate metabolism. For example, vitamin B1 is involved in the activation of transketolase, which neutralizes the toxic products of the sugar decomposition. In some cases, patients with diabetes mellitus have genetic deviations in the exchange of vitamins, so nutritional correction of the vitamin balance is an integral component of rehabilitation and prevention of diabetes mellitus complications.

When predicting the final result of the dietary supplements using in the production of meat products, analysis of the quantum chemical characteristics of the formulation components is necessary. The examination of changing in the molecular properties of lecithin, B1 and PP vitamins during the heat treatment was carried out in the Hyper Chem v.8 application by quantum chemical, semiempirical and molecular dynamic methods [3].

MATERIALS AND METHODS

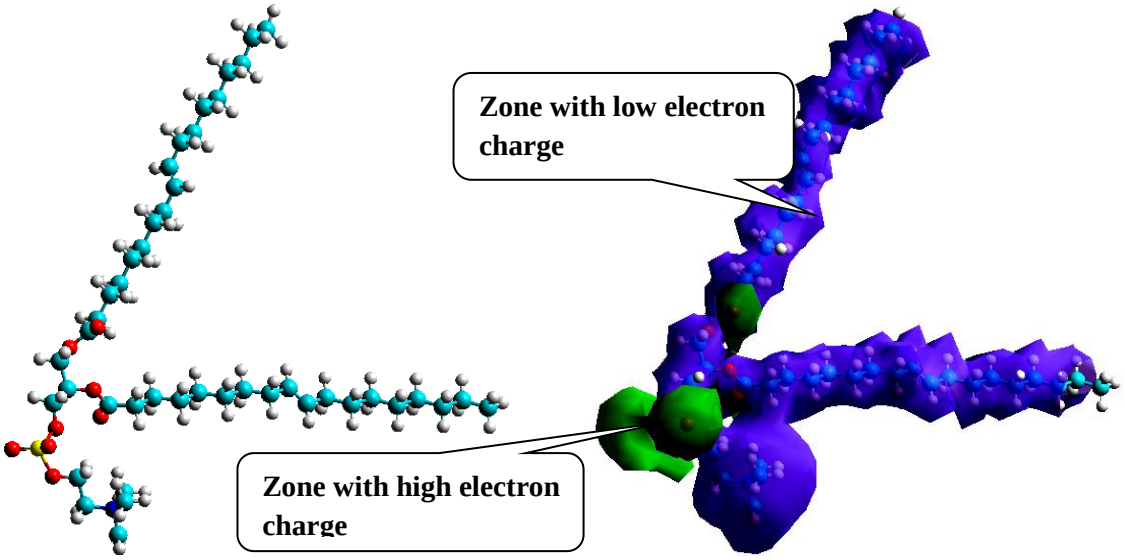
Meat raw materials as per GOST Standard (State Standard) 779-87, GOST 7724-77, lecithin (TU 9194-003-98925407-07), vitamins B1, PP (TU 64-5-71-91 – vitamin preparation) and other ingredients and materials meeting the requirements of the current regulatory documentation were used as research objects. To determine the quantitative content of vitamin B1 before and after heat treatment, a method based on the determination of the fluorescence intensity of thiochrome formed during the oxidation of thiamine after preliminary acid hydrolysis was used. The determination of vitamin PP was carried out by a method based on the formation of a colored derivative glutathione aldehyde. The amount of lecithin was controlled by the content of phosphorus in it. Photocolorimetric vandato-molybdate method with ammonium molybdate in the presence of molybdenum blue with preliminary ashing according to GOST 32903-2014 [3].The results of the experimental studies were processed using the Statistic v.10 b Statistic Neural Networks v.4 software packages [4, 5]. The modeling of molecules and the study of their properties were conducted using the Hyper Chem Release 8.01 software package [4, 5, 6].

RESULTS AND DISCUSSION

Since prophylactic dietary supplements are supposed to be used in food formulations, we will consider the possibility of using them in the technology of meat products, which provides for heat treatment. The technology of sausage production assumes a thermal treatment up to a temperature of 72° C in the center of the loaf. It is known that lecithin, vitamins B1 and PP are unstable to heat treatment by compounds, therefore

it is necessary to perform a stability analysis of the molecular structures of these components. At the initial stage, molecular structures of lecithin, vitamins B1 and PP were created, and their geometric optimization was performed using methods of molecular dynamics and quantum chemical calculations [4]. In Fig. 1A the structural formula of lecithin is shown. Evidence of the geometric optimization correctness, minimization of potential energy and the balance of the system energy properties was the total energy of the components under study (for lecithin -245735, for vitamin B1 -696169, for vitamin PP -32707.9 kcal / mol), the rms (Root Mean Square) gradients are approximated to zero value (for lecithin - 0.049, for vitamins B1 - 0.000 and PP - 0.075 kcal / (Å × mole). The dipole moments of lecithin, PP and B1 (9.681, 5.285, 1.999 Debye, correspondingly) characterize the irregularity distribution of the electron density. Using quantum-chemical and semi-empirical methods, the surface of the electrostatic potential distribution of lecithin (Fig. 1B) was investigated (similar studies were carried out for vitamins B1 and PP).

In addition to finding the minima of the potential energy surface corresponding to the stable states of the molecular system, it is of great importance to investigate saddle points, that are critical points of a different kind. In chemical kinetics, the saddle point on the potential energy surface between the region of state corresponding to the chemical reaction reagent and the stable state region of the chemical reaction products is considered from the standpoint of the transition complex theory. The activated complexes located in the saddle point don't give in to analysis to experimental investigation.



A B

A - is a structural model; B - is the distribution of the electron density on the molecule surface

Figure 1: Model analysis of a lecithin molecule

This is due to the fact that the lifetime of the molecular system in the state of the activated complex is extremely small. Under the influence of thermal fluctuations, the transition complex decays, and the system returns with a certain probability to a state of initial substances or to a state corresponding to stable reaction products. Therefore, quantum chemical calculation is practically the only source of information about molecular systems in transition states. The difference in the values of the potential energy at the saddle point and the minimum point is the activation energy, the value of which, within the framework of the transition complex theory, makes it possible to estimate the rate constant of a chemical reaction at a given temperature.

The modeling of the heat treatment process was carried out using the Brownian dynamics method. In Brownian dynamics, the action on the system under study is replaced by the effective frictional forces acting on each of its atoms and by random forces. In a period of time between two successive random effects, the atom moves under the action of forces from the other atoms of the molecule and the frictional force. The nature of the particle behavior resembles a sequence of random jerks, during which the particle moves under the action of gravity and the frictional force on the liquid side. Hence the name of the modeling method is Brownian or Langevin dynamics. To simulate the process of molecules thermal treatment, the Periodic boundary conditions

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module was used. The meaning of periodic boundary conditions in molecular dynamics is that with the help of this method the problem of whole system modeling is solved. Instead of solving an infinitely large number of differential equations corresponding to a macroscopic system, a periodicity cell that has finite dimensions is introduced. At the cell borders, the interaction potentials and atomic speed continue in a periodic manner. This means that if in the process of integration it is obtained that one of the particles of the system leaves the periodicity cell, then simultaneously an identical particle to it is added to the cell [4].

We put a molecule of lecithin in the Periodic boundary conditions, similarly we perform computer modeling for the molecules of vitamins B1 and PP. The results of the lecithin geometric optimization in the periodicity cell are shown in Fig. 2.

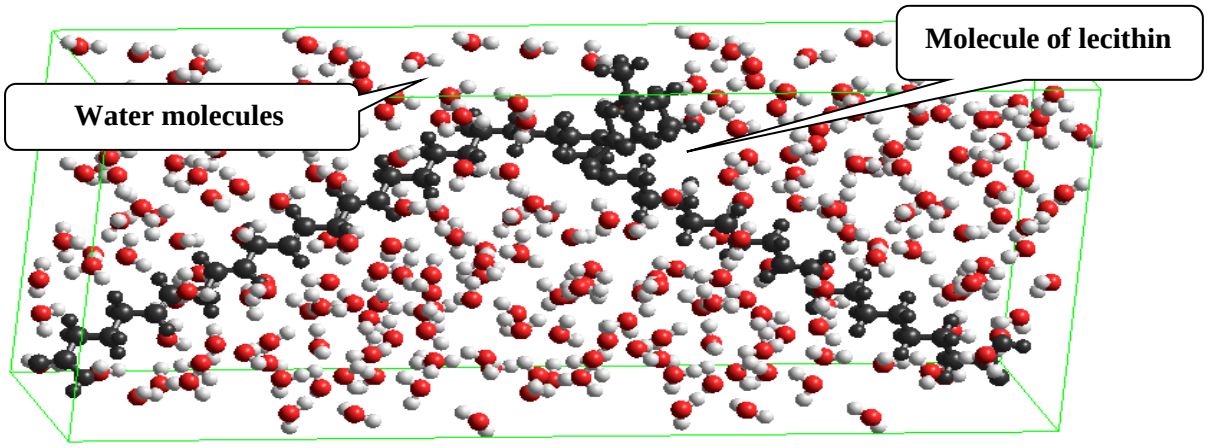

Figure 2: Model analysis of the lecithin heat treatment

The simulation of the heat treatment process was carried out until the energy state of the molecular system was stabilized (Fig. 3).

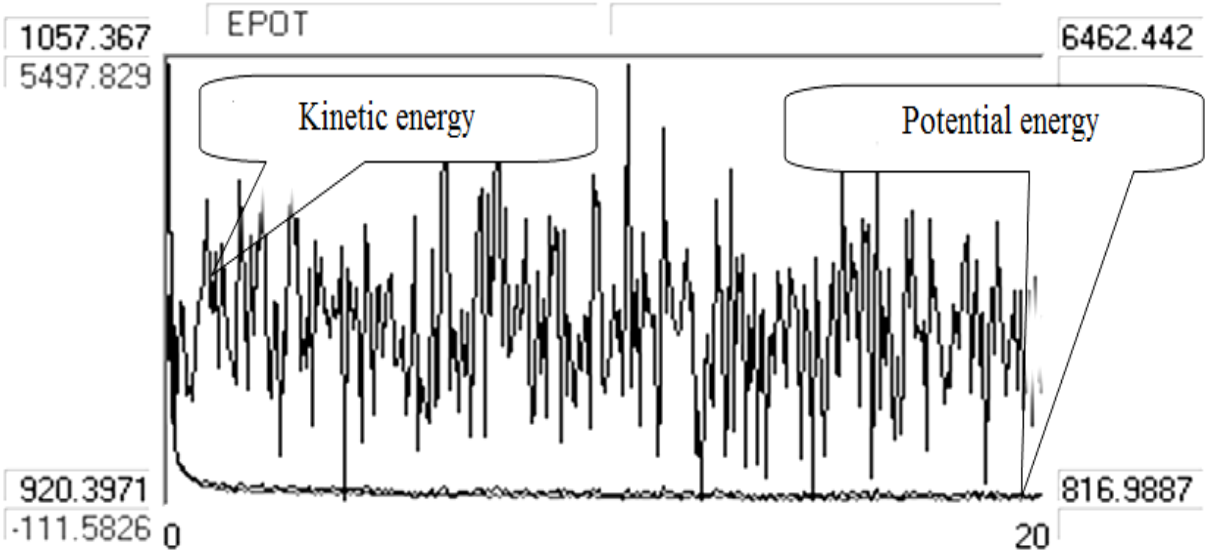

Figure 3: Changing the energy characteristics of the system during heat treatment

The stability of the energy state was determined from the fixed value (for a given period of time) of the potential energy value. The obtained graphical results (Fig. 3) indicate that under the using heat treatment conditions, the potential energy of the system has a stable value, which indicates a correctly performed procedure for modeling the technological process of heat treatment. Investigation of the molecular properties of lecithin, vitamins B1 and PP was conducted by quantum-chemical, semi-empirical and molecular-dynamic calculations (Table 1).

Table 1: Investigation of the molecular properties of lecithin, vitamins B1 and PP

Index	Energy, kcal / mol		
	Lecithin	Vitamin B1	Vitamin PP
Energy of activation	432,2	323,9	18,0
Change in the energy state of molecules during the heat treatment	425,1	22,1	19,7

From the data of Table. 1 it follows that the activation energy of a molecular system that is equal to the difference between the transition state energy and the geometric optimization energy for vitamin B1 and lecithin is higher than the changes in the energy state of these molecules (432.2, 323.9 as compared to 425.1, 22.1 kcal / mol, respectively), and for the vitamin PP it is lower - 18.0 against 19.7 kcal / mol. Consequently, the molecules of lecithin, vitamin B1 do not come into an excited state and do not change their structure under the using conditions of heat treatment. However, such temperature parameters can lead to a reduction of the quantitative content of vitamin PP.

The component composition of meat products includes a large number of ingredients (fats, proteins, carbohydrates, minerals, vitamins, etc.) that can influence the energy state of the system, therefore it is necessary to carry out experimental studies on the changes occurring with lecithin, vitamins B1 and PP in heat treatment time of the sausage product. The data on the changes in the quantitative content of dietary supplements used in the formulation (for a given significance level $q \leq 0.05$) are summarized in Table. 2.

Table 2: Change in the content of dietary supplements before and after heat treatment

Investigated components	Farcemeat	Ultimate product
	Quantitative content	
B1, mg /%	6,17	6,17
PP, mg /%	3,78	3,76
Лецитин, %	2,52	2,63

The results of Table 2 indicate that the change in the quantitative content of lecithin, vitamin B1 and PP in the product is insignificant and it is within the experimental error, therefore, with a given probability, it can be asserted that these heat treatment regimes do not contribute to the destruction of these components. It is important to note that the calculated amount of lecithin, introduced into minced meat, is 3 kg per 100 kg of basic raw materials, but in experimental studies the quantity in minced meat was 2.52%, and in the finished product it is 2.63%. This is due to the release of finished products (the addition of water to minced meat) and the presence of phospholipids in the feedstock. When studying the serum activity of blood marker enzymes in laboratory animals (rats) it was established that sausages do not have any toxic effect on the body and do not lead to an increase in cytolysis. Introduction in the diet of experimental animals with artificially induced diabetes meat products with recommended dietary supplements contributed to a decrease in glucose level by 8.48 mmol / l and an increase of the incremental rate in live weight in comparison with the group of animals that received only the basic diet.

CONCLUSION

The conducted analytical and experimental studies confirmed the expediency of using vitamins B1, PP and lecithin in the formulations for the production of food (subjected to heat treatment) for persons suffering from diabetes mellitus.

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