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Research Article

A NEW APPROACH OF GLUTEN DERIVATIVES FOR ACTIVITY AS THEORETICAL

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ABSTRACT

Gluten is the mainly rubbery mass that remains after wheat dough is being washed to remove starch granules and water-soluble constituents. Gluten is known as proteins and it plays an important role in indicating the unique baking quality of wheat. Their derivatives can be divided into two main fractions;: one of them is the soluble gliadins and the other is insoluble glutenins. After intaken gluten and monosodyum glutamate, the salt form of glutamate, the quantity of glutamate and glutamic acid in blood increases. In our study; we investigate the chemical properties of gluten ,glutamic acid and monosodyum glutamate as theoretical by using RHF/STO-3G method for quantum chemical calculations and geometry optimization methot to give direction the experimental studies as saving up time and money.
Keywords: Gluten, glutamate, glutamic acid, monosodyum glutamate, computational method.

1. INTRODUCTION

Gluten has a lot of proteins as monomers and polymers by linked disulphide bonds [1]. Gluten proteins play a key role in determining the unique baking quality of wheat [2]. Celiac sprue is a chronic disease suffered by approximately 1% of the world's population. The basis of celiac sprue is that an immune response to gluten happens in genetically susceptible individuals, leading to a series of malnutrition-related symptoms and even lymphoma in rare cases [3]. Glutamic acid was initially synthesized from wheat gluten. Recently, it has been produced by bacterial fermentation [4]. Monosodyum glutamate is the sodium salt of glutamic acid in some quantity in many natural food substances and as either an additive and flavor enhancer in many commercially packed food products and the liver plays an important role in the metabolism of glutamate. The consumption of MSG may result in varying degrees of liver and kidney injury, depending on the concentration applied [5]. After intaken of MSG ,there was highest glutamate in blood [6].Glutamate is an important neurotransmitterin the body has significant role in neuronal excitation [7]. On the basis of glutend its derivetives, results from this study indicated that the prevalence of glutamate in human methabolism had many important functions. The computational datas are important to understand th e chemical properties of Glutamate, Glutamic acid and Monosodyum glutamate.

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2. MATERIALS AND METHOD

The electronic structures of Glutamate, Glutamic acid and Monosodyum glutamate are studied by RHF/STO-3G method for quantum chemical calculations and geometry optimization. These methods and fully optimized geometric structure of the compounds of glutens derivatives by using this method were determined and evaluated [8,9]. Kuma010 has been studied experimentally and proved to be a promising gluten hydrolase under gastric conditions and the catalytic mechanism of it had been explained by the computational program.The computational free energy results are in reasonable agreement with the experimental data [10].

3. RESULTS AND DISCUSSIONS

The Glutamate, Glutamic acid and Monosodyum glutamate's values of ΔE, HOMO, LUMO, HOMO-LUMO gap and dipol moment are given in Table 1.

Table 1. The Glutamate, Glutamic acid and Monosodyum glutamate's values of ΔE, HOMO, LUMO, Δ (HOMO-LUMO) and dipol moment

RHF/STO-3G	Glutamate	Glutamic acid	Monosodyum glutamate
ΔE	-540.4103284	-541.34230511	-700.63800867
Dipol moment	1.8645	3.8435	8.3173
HOMO	0.02063	-0.31327	-0.17499
LUMO	0.52535	0.30120	0.32953
(HOMO-LUMO)	-0.50472	-0.614527	-0.50452

In Table 1; The energy levels of monosodyum glutamte is higher than glutamate and glutamic acid. Floris et al., emphasized that the glutamate ion in the zwitterionic form is more stable than the non-zwitterionic form comparing all the range of dielectric constants, while the glutamic acid is more stable in its non-zwitterionic form by using a computational method, density functional theory [11]. In our study; when we compared the polarity of Glutamate, Glutamic acid and Monosodyum glutamate as dipol moment; monosodyum glutamate is higher than the others so the solubility of it is best.

Jadhao and et al. indicated that a molecule having a small frontier orbital gap is more polarizable, is generally associated with a high chemical reactivity, low kinetic stability, and is called as soft molecule [12]. According to (HOMO-LUMO) gap; The stability of Glutamate, Glutamic acid and Monosodyum glutamate from high to low ;

Glutamic acid> Monosodyum glutamate> Glutamate

Glutamate has a high chemical reactivity, low kinetic stability than the other so ıt is more polarizable and soft molecule .

Glutamate acted as a neurotransmitter and it can decrease the development of autoimmunity and be effective role to protect from neuroinflammation so ıt may also have an important protective role and that its receptor may represent a therapeutic target [13].It is also an important receptor for learning and memory [14].On the other hand, excess glutamate in the brain may be a risk factor for brain disease and cognitive impairments [15].The highest level of it may also cause major depressive disorder [16].Moreover, its receptor of mGluR5 can cause epilepsy [17].

As indicated in literature; Glutamate has many functions and so glutamate's chemical properties are important to search its effects in methabolism.

The molecular structure of Glutamate is given in Figure 1.

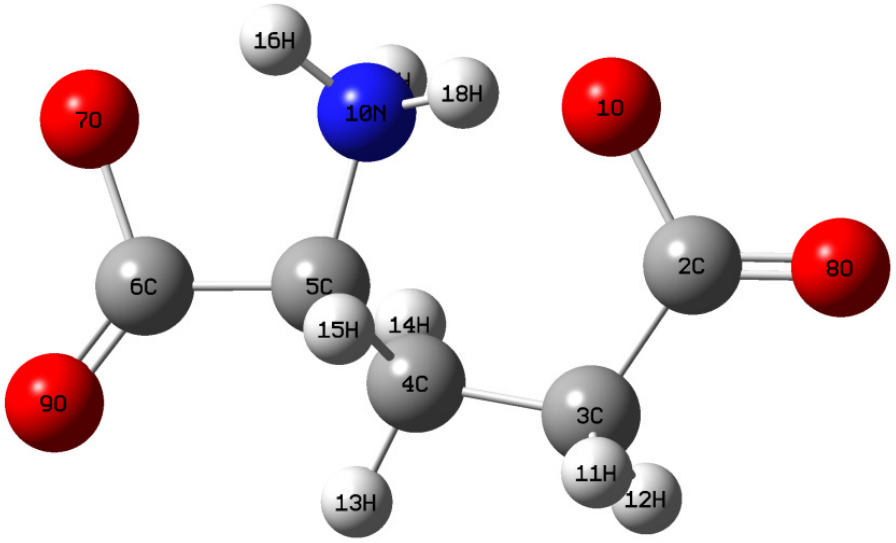

Figure 1. The molecular structure of Glutamate

The structure of Glutamic acid is given in Figure 2.

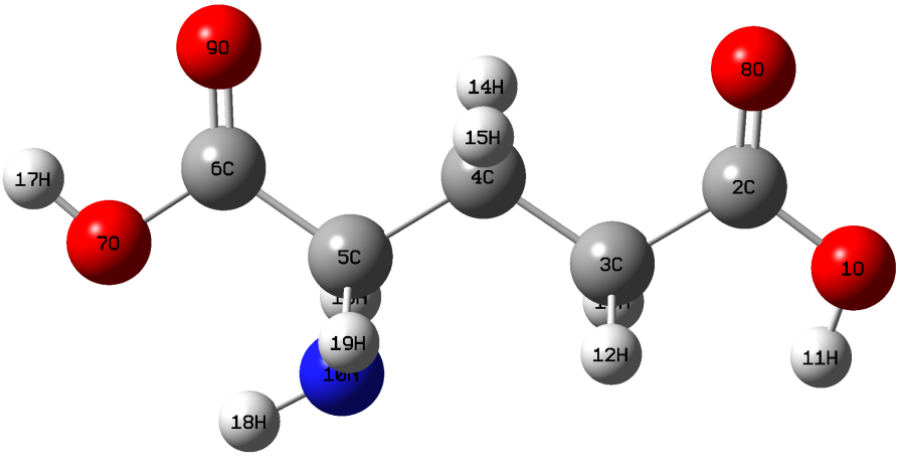

Figure 2. The molecular structure of Glutamic acid

The molecular structure of Monosodyum glutamate is given in Figure 3.

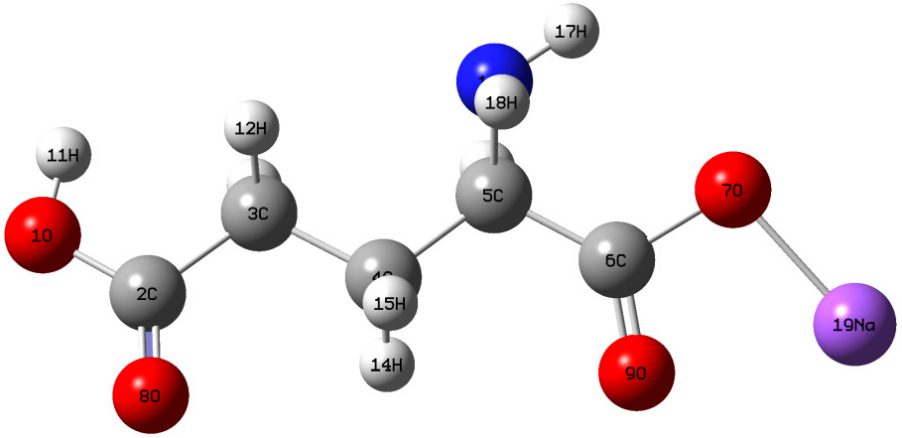

Figure 3. The molecular structure of Monosodyum glutamate

4. CONCLUSIONS

The chemical properties of Glutamate, Glutamic acid and Monosodyum glutamate can be explained by using computational method RHF/STO-3G in this study. The polarity of monosodyum glutamate is better and glutamate is more unstable according to the results of this computational method.The effects of glutamate and the other derivetives in brain the other tissues may be clarified by comparing the computational results and they can be used for experimental studies without time and matter consumption.

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