IN SILICO STUDY OF L-GLUTAMIC ACID AND L-GLUTAMINE FRAGMENTATION BY LOW ENERGY ELECTRONS

Laura Baliulyte[1], Jelena Tamuliene[2]

[1]Institute of Biosciences, Life sciences center, Vilnius University, Vilnius, Lithuania
[2]Institute of Theoretical Physics and Astronomy, Vilnius University, Vilnius, Lithuania
baliulyte.laura@gmail.com

Low-energy electrons are produced due to the interaction of X- and ϒ-rays with biomolecules. These low-energy electrons induce the damage of bioorganic molecules including amino acids e.g. L-glutamic acid (Glu) and L-glutamine (Gln).

It is well know that, L-glutamic acid is the most abundant intracellular amino acid (concentrations 2-20 mM) whereas L-glutamine is the most prevalent extracellular amino acid (concentration 0.7 mM) [1]. Furthermore, the mass of these amino acids is very similar- Glu (m=147 Da), whereas Gln (m=146 Da). While side chains of these amino acids are quite different: L-glutamic acid R is $(CH_2)_2$–COOH, whereas L-glutamine- $(CH_2)_2$-$CO(NH_2)$. According to our knowledge, there is no data about Glu and Gln fragmentation similarities and differences.

The aim of our study is to determine whether the chemical composition and appearance energies of same mass fragments, which are produced during the fragmentation of Glu and Gln by low energy electrons, are different.

We used Gaussian 09 Rev D.01 program. Structures and fragments of the L-glutamic acid and L-glutamine molecules were studied by B3LYP with cc-pVTZ. Fragments were selected on the basis of the experimental mass spectrometry data. We used L-glutamic acid and L-glutamine positively charged fragments mass spectrum measured by our colleagues (L. Romanova, V. Vukstich, A. Papp and A. Snegursky) [2] and data from the NIST database [3]. Peaks at masses m/z=28, 41, 56 and 84 are most intensive in Glu and Gln mass spectrums. Moreover, their intensities are similar.

Our research indicate that CH_2N^+ (m/z=28) and $C_3H_5^+$ (m/z=41) cations could be produced during fragmentation of both Glu and Gln, while $C_3H_6N^+$ (m/z=56) and $C_4H_6NO^+$(m/z=84) could only be produced during fragmentation of Glu, $C_2H_2NO^+$(m/z=56) and $C_4H_8N^+$(m/z=84)- only during fragmentation of Gln.

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