A study on the influence of water on the L-isoleucine fragmentation

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Low-energy electrons are produced due to the interaction of X/gamma rays with biomolecules. These low-energy electrons cause damage of molecules, including amino acids, e.g. isoleucine. L-isoleucine is important for blood sugar regulation, muscle development and repair. Nevertheless, information on L-isoleucine fragmentation is insufficient. Most biophysical processes (also amino acids fragmentation) occur in water. Data on the fragmentation of amino acids in water are scarce, although they are relevant to the analysis of processes in organisms. Our research is performed aiming to determine the influence of water to the process of fragmentation of isoleucine. We used density functional theory B3LYP method and cc-pVTZ basis to evaluate the energy of appearance of the positively charged fragments. Polarizable continuum model is used to evaluate the presence of water. We applied Gaussian 03 Rev D.01 program. Cations for study were selected on the basis of the experimental data of mass spectrometry published in the NIST database. The most intensive peaks in the mass spectrum of L-isoleucine correspond to m=86 a.m.u., 75 a.m.u. and 30 a.m.u. We determined that fragment with mass 86 a.m.u. is $C_5H_{12}N^+$, m=75 a.m.u.- $C_2H_5NO_2^+$, m=30 a.m.u.- CH_4N^+. Energy of appearance of $C_5H_{12}N^+$ is equal to 8.85 eV, of $C_2H_5NO_2^+$- 9.48 eV, of CH_4N^+- 10.01 eV in vacuum, while in water- of $C_5H_{12}N^+$ - 9.76 eV, of $C_2H_5NO_2^+$- 10.32 eV, of CH_4N^+- 10.86 eV.

In conclusion, more energy is needed for the formation of identical fragments in the water.

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Biography

Laura Baliulyte is a PhD student in the Institute of Biosciences, Life Sciences Center, Vilnius University. Fields of research: theoretical modeling of amino acids fragmentation, biochemical reactions, biophysical processes. She is co-author of several articles. Corresponding email: baliulyte.laura@gmail.com