

# MASS SPECTROMETRY, PROTEOMICS AND POLYMER CHEMISTRY

May 20-21, 2019 | Rome, Italy

Baliulyte L et al., J Chem Tech App 2019, Volume 3

## A STUDY ON THE INFLUENCE OF WATER ON THE L-LEUCINE FRAGMENTATION

**Baliulyte L and Tamuliene J**

Vilnius University, Lithuania

All living organisms are constantly affected by ionizing radiation emitted by natural sources such as cosmic rays and radionuclides contained in rocks from the Earth, food, water and air etc. Moreover, ionizing radiation exposures also occurs during medical procedures. Low-energy electrons are produced due to the interaction of X- and Y rays with organic molecules. These low-energy electrons cause damage of biomolecules, including amino acids, e.g., Leucine. Data on fragmentation of amino acids in water are scarce, although they are relevant to the analysis of processes in living organisms. Hence, the aim of the author's research is to determine whether the appearance energies of fragments differ between conditions with and without the influence of water included. They used density functional theory (DFT) B3LYP method and cc-pVTZ basis set. The polarized continuum model (PCM) method was used to evaluate the presence of water. They applied Gaussian 03 Rev D.01/09 Rev D.01 program. Fragments were selected based on the experimental mass spectrometry data in the NIST database. The strongest peaks in the mass spectrum of L-leucine correspond to  $m=86$  amu, 44 amu and 30 amu. They determined that cation with mass 86 amu is  $C_5H_{12}N^+$ , cation with mass 44 amu is  $CO_2^+$  and cation with mass 30 amu-  $CH_4N^+$ . The results of author's research with and without the influence of water indicate that more energy is needed for the formation of same cations in water.

## BIOGRAPHY

Laura Baliulyte is a PhD student at the Institute of Biosciences, Life Sciences Center, Vilnius University, Lithuania. Her area of research mainly focuses on theoretical modelling of amino acids fragmentation, biochemical reactions and biophysical processes. She is the co-author of several articles.

[baliulyte.laura@gmail.com](mailto:baliulyte.laura@gmail.com)



Note: