Contribution ID: **250** Contribution code: **S13-BMP-100** Type: **Oral presentation**

Non-supervised algorithms for Raman spectral decomposition in the in-vitro study of oxide nanoparticles effects on human cells

Thursday, 1 September 2022 11:45 (15 minutes)

Study of the effect of inorganic nanoparticles on the human cells has been intensified due to emerging applications of such nanoparticles in diagnostics, drug delivery, medical therapy, etc [1]. Several classes of nanoparticles have been proposed for use in cancer therapy as they were demonstrated to decrease cancer cells viability in the scientific studies. Nanoparticles that have so called dual effect, diminishing the cancer cell numbers but preserving the healthy cells are of importance here since this is the primary criterion for application of nanoparticles in living organisms.

Raman spectroscopy has a potential to be used for in-vitro study of integral biomolecular changes induced in the cells by treatment with different chemicals or resulting from a particular disease [2,3]. Cellular Raman spectra contain vibrational modes characteristic for different biomolecules with a high degree of overlapping. Various multivariate algorithms can be applied to deduce small spectral changes in the spectra of cells in abnormal states [2]. Supervised multivariate algorithms are mainly used for classification of cancerous or other abnormal cells and their separation from the healthy ones, hiding the information about the nature of the differences that the classification model is built upon. On the other hand, unsupervised algorithms can be used for detection of spectral changes that can be correlated with specific biomolecular changes.

We have used standard principal components analysis (PCA), non-negative PCA and non-negative matrix factorization (NNMF) methods to decompose Raman spectra of the cancerous HeLa cells and healthy fibroblast MRC-5 cells into spectral components. Whereas PCA produces components expressing highest degree of spectral variance, non-negative PCA and MF components are more closely related to the Raman spectra of the individual cell molecules that are more abundant.

Spectra of several cell sets were analyzed, each of the sets containing untreated cells and cells exposed to the oxide nanoparticles of CeO2 and ZnO for several nanoparticle concentrations. Decrease of DNA content, changes in lipid-to-protein ratio and in lipid saturation degree are some of the processes that were possible to follow based on the behavior of certain spectral features contained within algorithm-obtained spectral components, acting as markers. Spectral decompositions obtained with non-negative algorithms for particular cell types and particular nanoparticles were cross-compared and combined in order to obtain more general model for the assessment of the magnitude of nanoparticle-induced changes in the cells.

References

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Session Classification: S13 Biophysics and Medical Physics

Track Classification: Scientific Sections: S13 Biophysics and Medical Physics