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SOM-assisted analysis of fluorescence spectroscopy data for the search of life

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Abstract –The search for life in the Universe as well as the understanding of the life phenomenon belong to the highest priority goals of astrobiology and is therefore addressed in most of space missions. The existing scientific uncertainty of the term "life" makes this task extremely challenging. The main goal of this study was to investigate the potential of the 3-D fluorescence spectroscopy accompanied by a self-organizing map (SOM) approach for the detection of (life-specific) substances in terms of both specificity and sensitivity. A similar approach has been already successfully used for the monitoring of river organic matter and diesel pollution [1].

In our work first we recorded excitation-emission matrices (EEMs) of different substances using fluorescence spectroscope Jasco FP-8500 (Fig.1, 2). Then, the obtained spectroscopic fingerprints of various organic and non-organic molecules were analyzed and systematized. In particular, a focus was made on various sulfur compounds substances that can be important indicators for the presence of living organisms [2]. For analyzing organic molecules a suspension of living Proteobacterium *Thiobacillus thioparus* cells was prepared. This chemoautotroph microorganism depends on sulfur and therefore can be taken as an example for chemoautotroph organisms living in deep water marine environments.

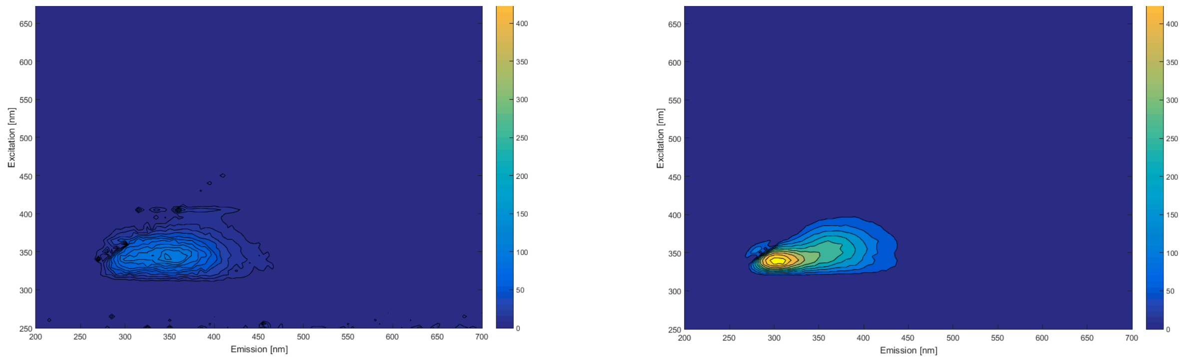

Fig 1. Excitation-emission matrices for sodium sulfide: 0.01 M (left) and 0.1 M (right)

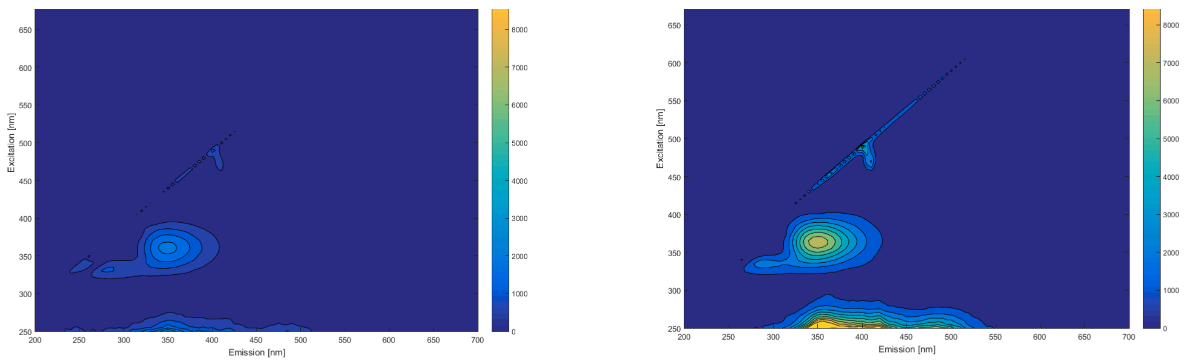

Fig 2. Excitation-emission matrices for living *Thiobacillis thioparus* cells, EEM Fluorescence Spectroscopy data at day 3 (left) and day 9 (right) One can see the increase in fluorescence-intensity due to the larger amount of cells.

The following step was devoted to a deeper analysis and systematization of the obtained data. A common tool for analyzing EEMs is parallel factor analysis (PARAFAC) [3]. Another interesting approach is the application of artificial neural networks (ANN). SOMs, being capable to non-supervised learning, represent an ANN-variant that is very promising for future autonomous applications [4]. For the SOM-assisted data analysis, different “toolboxes” have been already developed, including the most important algorithms called “SOM-Toolbox” [5] and “DOMFluor toolbox” [6]. Nevertheless, the collected EEM data needs to be imported and preprocessed in a certain way to match the criteria for the toolboxes. For this purpose a MATLAB Import and Preprocessing toolbox has been created by us. After the preprocessing the EEM data are fed into the SOM and analyzed in an autonomous fashion (Fig.3).

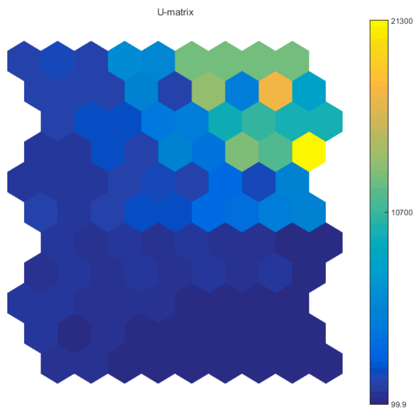

Fig 3. An example pf the SOM-assisted processing (U-map) of the EEM data collected for inorganic compounds at different concentrations

A big advantage of the SOM that we are trying to realize practically is that the SOMs allow self-learning automatic recognition and differentiation between multiple classes of substances and therefore are particularly useful as a tool for detection and interpretation of life signatures by an autonomous probe.
Further on the data could be also used for navigation purposes, for instance, for navigating an autonomous underwater vehicle by a method similar to a chemotaxis.

References

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