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NEURAL NETWORK FOR REACTION-DIFFUSION SYSTEM IMAGE ANALYSIS

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Abstract. To evaluate the encapsulation process of active molecules into supramolecular assemblies one proposed to use image analysis. Two convolutional neural networks were proposed to obtain a high validation accuracy and a specific confusion matrix.

There are several trends in chemistry that are based on biomedical application. One of them is encapsulation of active molecules into complex chemical structures such as supramolecular assemblies. These assemblies consist of two or more compounds held together by non-covalent bonding. One of the most well-known supramolecular structures is melamine cyanurate.
Melamine and cyanuric acid molecules are linked by hydrogen bonding into several structure forms such as continuous linear structure and cycle rosette. Rosette structure form provides a possibility of encapsulation of large organic molecules into melamine cyanurate. The chosen compound is TAMRA-DNA. One decided to use agar gel to provide diffusion control of the encapsulation process. The luminescence of the obtained capsules greatly depends on the amount of Mg^{2+} ions that is confirmed by optical microscopy method.
The aim of the research was to develop an analysis system to evaluate the concentration of different compounds in the capsules. The form of capsules and the intensity of yellow luminescence is difficult to differ by human vision, thus neural network is used instead. The dataset consists of five categories that include images with specific concentration of Mg^{2+}. There are more than one thousand images after augmentation in every category. After the dataset preparation stage there is a neural network learning. Two different convolutional neural networks were used to find image patterns for different concentration. The validation accuracy for the first neural network is 81%, however the confusion matrix shows mistakes for several concentrations of magnesium ions. The second neural convolutional network VGG16 has the validation accuracy about 96% with such a good confusion matrix.
The research results confirm that convolutional neural networks can be used for reaction-diffusion system image analysis. It may increase the analysis process and avoid operator's mistake. Thus, the next step of the research is to define the concentration of TAMRA-DNA by the neural networks to evaluate the encapsulation process.

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