Abstract

Diploma thesis deals with expanding the artificial intelligence DeepReI with the prediction of retention indices of substances in gas chromatography for standard non-polar and polar stationary phases.

The theoretical part describes artificial intelligence, convolutional neural networks, and the principles of neural network learning. There is also a brief overview of the applications of neural networks in analytical chemistry.

In the experimental part, the original DeepReI model was extended to predict the retention indices of substances for standard non-polar and polar stationary phases. Furthermore, more accurate predictions of retention indices were achieved for semi-standard non-polar stationary phases compared to existing models. The applicability of the model for substance identification was verified through non-targeted analysis of non-alcoholic beers using gas chromatography with mass detection.