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Quick learning algorithm of self-organizing map using an index layer and its application to similar structure mapping of chemicals

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The authors have been investigating adaptable chemical structure information handling and its applications for chemical data mining. This paper describes a quick learning algorithm for Self-Organizing Map (SOM) using an Index Layer for data visualization of TFS data space as one of the data mining techniques. Searching for the Best Match Unit (BMU) on a competition layer of SOM is quite time consuming when the large number of neurons are set on the layer. For this problem, an “index layer”, that is located between input layer and competition layer, is introduced to quickly find a location area of BMU on the competition layer. The algorithm was implemented and tested with 1354 dopamine antagonists. Its computational time was shortened to approximately 1/9 in comparison to normal method.