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PREDICTION OF THE TOXICITY OF SOME AROMATIC COMPOUNDS BY NEURO-FUZZY METHOD

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Abstract

In recent years, the neuro-fuzzy systems have drawn increasing research interest. This approach has been successfully used in various areas, such as natural language understanding, robotics, and medical diagnosis, particularly based on neuro-fuzzy networks. The aromatic compounds form a large and structurally diverse group. These are interesting from a toxicological point of view since they elicit a number of toxicities to different species. A set of about 21 descriptors was examined. They were calculated using an original algorithm taking into consideration chemical composition and main structure aspects for 71 organic compounds benzene derivatives, without other cyclic structure. Constitutional descriptors are used according to CODESSA (Katrizky, 1994): through quantitative rapport between constitutive elementary species and molecular mass and the type of bonds involved. The problem is modeled with the original developed system NIKE: Neural explicit&implicit Knowledge inference systEm is a hybrid intelligent system developed for prediction, based on modular neural and neuro-fuzzy networks. The contribution of each descriptor for their influence in toxicity was measured. Consequently, models for the reduced data sets were developed. The initial data set was split in normalized equally distributed 4 classes. The idea is to insert in the hybrid intelligent system NIKE, the explicit knowledge about classes (specific QSAR forms) as equivalent fuzzy rules, as well as the trained models. The neural models are more sensible to the noisy data, which make them a very important indicator of the significance of the descriptors to toxicity. This conclusion recommends it as suitable for toxicity prediction task. Future work will be carried out following the outlined possibilities of neural and neuro-fuzzy integration with explicit QSARs into the hybrid system NIKE.

Keywords: toxicity prediction, aromatic pesticides, neuro-fuzzy method

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