Title of Research:

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Sophisticated hazard prediction by active QSAR modeling

Principal Investigator:

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Summary of Research:

In the preceding study, we obtained successful results about data predictions by the PLS modeling with the active sampling which was based on structure similarity for making a set of training data. In this study, according to the active QSAR modeling approach to the data prediction, we have developed a computer system for the eco-toxicity prediction of chemicals, which automated a whole process of the input of query structure , active sampling of training compounds that have similar structures to the query, computation of the PLS model, prediction and display of the toxicity of interest. The user can use the system without the use of keyboard input. Following three aspects is an important basic concept in the development of this system; 1) System that the user wants to use, 2) that is easy-to-use for the user, 3) that is useful for the user. In this study, in addition to the automation of the whole process described above, we have developed a structure editor, and additional tools for calculation of molecular formula and molecular weight calculation. We have implemented a computer program for logP estimation which is based on the group contribution method, to the system. The performance of the system that was developed in the study was evaluated through the prediction experiment with external data. These results were also compared with the results of other systems (ECOSAR and KATE).

Timeline:

1st Nov. 2013 – 28th Feb. 2015

Topics:

Poster presentation and system demonstration at The Second New LRI Workshop, Tokyo, Aug., 2014

Publications:

1) Yuji Ikegami, Yoshimasa Takahashi, **Prediction of eco-toxicity of chemicals using atomic fragments: Prediction of fish toxicity (96h-LC50)**, Proc. of the 23rd Symposium on Environmental Chemistry, 2014, May, Kyoto.
2) Yoshimasa Takahashi , Mika Ohyama and Tomoya Yamazaki, **Active QSAR modelling for environmental toxicity prediction of chemical substances**, 20th EuroQSAR, Saint-Petersburg, Russia, Sep. 2014.
3) Yuji Ikegami, Yoshimasa Takahashi, **Fish toxicity prediction of chemicals using atomic fragment method: Grobal parameters and chemical group parameters**, Proc. of the 42nd Symposium on Structure-Activity Relationships, 2014, November, Kumamoto.
4) Yoshimasa Takahashi, Tomoya Yamazaki, Mika Ohyama, Yuji Ikegami, **Sophisticated hazard prediction by active QSAR modeling**, Proc. of the 27th annual meeting of the Japanese Society for Alternatives to Animal Experiments, 2014, December, Yokohama.