***Title of Research:***

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# Sophisticated hazard prediction by active QSAR modeling

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***Summary of Research:***

For this year, we have continued to develop the desk-top software tool, ToxCalc, which can be used for the eco-toxicity prediction of chemicals by means of the active QSAR modelling reported in our preceding work. Our points of the development of this tool are as follows; 1) System that the user wants to use, 2) system that is easy-to-use for the user, 3) system that is useful for the user. The user can use the Tox-Calc without any keyboard input. The system fully automated all the process of input a query structure, the active sampling of training compounds, making a QSAR model and the prediction of the specified toxicity. We have prepared the databases of three different endpoints, fish acute toxicity (96h-LC50), daphnia acute toxicity (48h-EC50) and algae growth rate (72h-EC50), which are used to collect the training compounds similar to the query and to make a QSAR model with those data. We have also implemented several additional functions to the system; searching for the experimental toxicity data by CAS number, referring to the QSAR information of the current prediction model, and setting the user preference of the system parameters for the prediction.

***Timeline:***

1st Mar. 2015 – 29th Feb. 2016

***Topics:***

Tox-Calc system demonstration at LRI Workshop 2015, Tokyo, Aug., 2015

***Publications:***

1）Yoshitaka Inagaki, Tomoya Yamazaki, Yoshimasa Takahashi, “Environmental toxicity prediction using active QSAR modelling”, The 24rd Symposium on Environmental Chemistry, Sapporo, Jun., 2015.<in Japanese>

2）Yoshitaka Inagaki, Tomoya Yamazaki, Yoshimasa Takahashi, “Development of a desk-top tool ToxCalc for eco-toxicity prediction of chemicals”, The 43rd Symposium on Structure-Activity Relationships and The 10th Japan-China Joint Symposium on Drug Discovery and Development、Niigata、Sep., 2015.

3）Yoshitaka Inagaki, Tomoya Yamazaki, Yoshimasa Takahashi, “Desk-top tool for eco-toxicity prediction of chemical substances”, The International Chemical Congress of Pacific Basin Societies 2015, Honolulu, Dec, 2015.