

**Title of Research:**

16\_S01-01-2

**Advanced system development for the hazard prediction and the environmental risk assessment/management of chemical substances**

**Principal Investigator:** Bin-Le Lin, Chief Senior Researcher, Research Institute of Science for Safety and Sustainability, National Institute of Advanced Industrial Science and Technology. 16-1 Onogawa Tsukuba City, Ibaraki, 305-8569 Japan. (Tel) +81-29861 8844, (e-mail) [binle-lin@aist.go.jp](mailto:binle-lin@aist.go.jp); Yoshimasa Takahashi, Professor of Toyohashi University of Technology. (Tel) +81-532-446878, (e-mail) [taka@cs.tut.ac.jp](mailto:taka@cs.tut.ac.jp);

**Summary of Research:**

In this research, collaboration between AIST and Toyohashi University of Technology will develop an advanced system to enable risk assessment management of unconfirmed existing chemical substances and new substances without hazard information faced by Chemical Industry Association. Toward the goal of designated research, the following research outputs were obtained. 1) Improvement and expansion of hazard DB for PEACH-QSAR system development, and were installed in MeRAM Ver. 2.0; (2) We examined functions and specifications for the data automatic export for PEACH-QSAR system development and start to develop the interface; (3) We examined functions and specifications for connection with KATE and started to develop interfaces; (4) External interface for connection with PEACH-QSAR system was studied, and design and development on detail specifications were carried out; (5) Updated and improved existing functions (effective risk management measures, compliance with the CSCL etc.), and released a new version of MeRAM (Japanese version and English version); (6) We disseminated the tool and Japanese style management of chemicals (CSCL), and hosted an education session of MeRAM at Awajishima ICCA-LRI Workshop, and presented on SETAC meetings. In addition, we accepted student of Toyohashi University of Technology for 2 months (January 9 to February 23, 2017), collaborated on DB analysis of MeRAM and DB creation for PEACH development.

**Timeline:**

From March 2016 to February 2017

**Topics:**

None

**Publications:**

- 1)(Presentation at Domestic Meeting) The 26th Environmental Chemistry Debate (7-9 June 2017), Shizuoka Convention Center, Shizuoka, "IT solution for Cumbersome Ecological Risk Assessment and Management of Chemicals: AIST-MeRAM".
- 2) (Invited Speech at Domestic Workshop) Research Committee on Safety Assessment Winter seminar in 2016: "Ecological risk assessment of chemical substances in water environment". December 3, 2016. Jinbocho Mitsui Building, Tokyo.
- 3) (Paper Publication) Institution magazine "Toxicity Inquiry Box" of the Safety Assessment Committee, 2017: "Ecological risk assessment of chemical substances in water environment".
- 4) (Presentation at International Meeting) The SETAC North America 37th Annual Meeting, Orlando, Florida, United States. 7-11 November 2016. Oral presentation An all-in-one ecological risk assessment (ERA) tool: AIST-MeRAM.
- 5) (Research Outcome Exhibition) AIST Techno Bridge Fare, 20-21 October 2016, Tsukuba. IT solution for Cumbersome Ecological Risk Assessment and Management of Chemicals: AIST-MeRAM.
- 6) (Presentation at International Meeting) The SETAC A/P Conference 2016, Singapore, 14-20 September 2016. A Free Tool (AIST-MeRAM Ver. 2.0) for Multi-purpose Ecological Risk Assessment and Management of Chemicals, Oral presentation.



## Development and assessment of new risk assessment methods

- 7) (Presentation at PCD, TISTR, NSTDA) Workshop on Japan-Thailand Bilateral Cooperation on Chemical Management, 3rd-7th October 2016, Bangkok, Thailand.
- 8) (Invited Speech at Thailand) Risk Assessment of Chemicals. Symposium Capability Building for OECD Guideline for Testing of Chemicals and Ecotoxicology in ASEAN, hosted by Thailand Institute of Scientific and Technological Research (TISTR) & Ministry of Science and Technology (MOST) of Thailand, Chaophya Park Hotel, Bangkok Thailand, 8-9 Aug 2016.

**Title of Research:**

16\_S01-01-2

**Advanced system development for the hazard prediction and the environmental risk assessment/management of chemical substances**

**Subtitle: Development of the sophisticated basis tool environmental hazard prediction**

**Principal Investigator:**

**Yoshimasa Takahashi, PhD (Professor, Dept. Comp. Sci. Eng., Toyohashi Univ. Tech.)**

1-1 Hibarigaoka, Tempaku-cho, Toyohashi 441-8580 JAPAN

(tel)+81-0532-44-6878, (email)taka@cs.tut.ac.jp

**Collaborators:**

Tetsuo Katsuragi (Assit. Prof., Toyohashi Univ. Tech.)

Dai Furukawa (Graduate student, Toyohashi Univ. Tech.)

Taku Izumihara (Graduate student, Toyohashi Univ. Tech.)

**Summary of Research:**

For this year, in order to take a good collaboration with PEACH, which is a desk-top tool for eco-toxicity prediction of chemicals by means of active QSAR modelling, we have constructed a dictionary of chemical structures for the MeRAM because the MeRAM have no chemical structure information excepting chemical name and CAS registry number. The dictionary tool involves the data search functions by CAS number, compound name, molecular formula, full structure search and similar structure search.

We also have investigated the availability of group contribution method based on atomic fragments for fish toxicity prediction of chemical substances. The atomic fragments were originally defined by Viswanadhan et al. in their study on the prediction of molecular properties of logP and molar refraction. To predict the fish toxicity we employed the set of atomic fragments, and determined the toxic fragment constants to the individual atomic fragments with a set of experimental toxicity data of 366 compounds. The toxicity constants gave successful results to the fish toxicity prediction. Alternatively, we investigated estimation of an aqueous solubility parameter (logS) using the atomic fragment method. Those contributions of individual fragments to the logS were determined with the experimental values of 1290 compounds by simplex optimization technique. Five-fold cross validation test gave us the prediction accuracy of the RMSE of 0.73 for the present dataset.

**Timeline:**

1<sup>st</sup> Mar. 2016 – 28<sup>th</sup> Feb. 2017

**Topics:**

Poster presentatikon at ICCA-LRI International Workshop 2016, Awaji, Jun., 2016

**Publications:**

- 1) Dai Furukawa, Yuji Ikegami, Tetsuo Katsuragi, Prediction of Fish Toxicity of Chemicals by Atomic Fragment Method: Refinement of hetero atom fragments and optimization of the fragment constants, JSAI2016, Kitakyushu, Jun., 2016.
- 2) Yoshimasa. Takahashi, Yoshitaka Inagaki, Tetsuo Katsuragi, 21st European Symposium on Quantitative Structure-Activity Relationship (EuroQSAR), Verona, Sep., 2016.
- 3) Dai Furukawa, Tetsuo Katsuragi, Yoshimasa Takahashi, Fish toxicity prediction of chemicals using atomic fragment method: refinement of the fragments and improvement of the prediction



Development and assessment of new risk assessment methods model, The 44th Symposium on Structure-Activity Relationships, Kyoto, Nov., 2016.