

**Title of Research:** 16\_S01-01-2

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

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**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) MeRAM Ver.2.0 as the latest released version (Japanese version & English version) were open for public; (2) added a function to MeRAM that can automatically export the built-in data of MeRAM according to various purposes of users; (3) In order to be used by environmental administration, a function that can automatically launch KATE from the interface of MeRAM, and then can automatically acquire the predicted value of KATE and use it for risk assessment; Although the release of the MeRAM latest version equipped with the functions of 2) and 3) is not yet available, it was distributed to many participants at seminars of the Ministry of the Environment and workshops organized by AIST; (4) Started to develop our own methodology for predicting the toxicity of chemical substances from October of last year. Based on various fingerprint information (structure and physical information) of chemical substances and toxicity information, toxicity estimation by machine learning but not using QSAR equations is under developed.

**Timeline:** From March 2017 to February 2018

**Topics:** None

### **Publications:**

- 1) (Paper Publication) Institution magazine "Toxicity Inquiry Box" of the Safety Assessment Committee, 2017: "Ecological risk assessment of chemical substances in water environment".
- 2) (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".
- 3) (Invited Speech at Domestic Workshop) The 26th Environmental Chemistry Debate (7-9 June 2017), Shizuoka Convention Center, Shizuoka, "Open Science in Environmental Chemistry" Why do not open your own data: Potential of using open data."
- 4) (Presentation at Domestic Meeting) The 20th Water Environment Symposium (26-27 September 2017), Wakayama University, "Hierarchical ecological risk assessment and management of chemical substances using MeRAM".
- 5) (Presentation at Domestic Meeting) The Tougou-no-hi-no Symposium (4-5 October 2017), Tokyo University, "Attempt to utilize integrated database for environmental risk assessment and risk communication of chemical substances".
- 6) (Presentation at Domestic Meeting) The 30<sup>th</sup> Annual Meeting of Japan Risk Research (27-29 October 2017), Shiga University, "Risk assessment of toxicity deficient substances by linking MeRAM and KATE".
- 7) (Invited Speech at Domestic Workshop) Environmental Science Seminar hosted by Ministry of the Environment Seminar on chemical substance environment survey (15-16 January 2018), Tokyo, "What MeRAM can do."
- 8) (Invited Speech at Domestic Workshop) MeRAM Workshop hosted by AIST (23 January 2018),



Development and assessment of new risk assessment methods

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## **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:**

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

Mitsuru Sato (Graduate student, Toyohashi Univ. Tech.)

Tsubasa Ishikawa (Graduate student, Toyohashi Univ. Tech.)

**Summary of Research:**

In this fiscal year (Fiscal 2017) research, we designed external file specifications for data import to PEACH(Prediction of Environmental Affect of Chemicals) with the aim of utilizing external data, and implemented the import function of external data utilizing the chemical structure dictionary. For the chemical structure dictionary tool developed in the previous year, we expanded the data import function and revised the user-interface for strengthening cooperation with MeRAM. In addition, we refined the estimation model of water solubility parameter logS by atomic fragment method. We developed an estimation model of vapor pressure too. On the other hand, for the short-term toxicity (96h-LC50) against fish, we developed alternative prediction models based on quantitative activity-activity relationships (QAAR) for the toxicity tests with different fish species. The results show that the QAAR models would be very useful for prediction of missing data.

**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) Tsubasa Ishikawa, Tetsuo Katsuragi, Bin-Le Lin, Yoshimasa Takahashi, Studies on complementation of missing data of fish toxicity by Quantitative Activity-Activity Relationship, 26th Symposium on Environmental Chemistry, Shizuoka, 2017.
- 2) Taku Izumihara, Tetsuo Katsuragi, Bin-Le Lin, Yoshimasa Takahashi, Construction of Chemical Structure Dictionary for MeRAM, 26th Symposium on Environmental Chemistry, Shizuoka, 2017.
- 3) Mitsuru Sato, Dai Furukawa, Tetsuo Katsuragi, Yoshimasa Takahashi, Prediction of Aqueous-Solubility Using an Atomic Group Contribution Method, 26th Symposium on Environmental Chemistry, Shizuoka, 2017.
- 4) Yoshimasa TAKAHASHI and Ryota KIKUCHI, Algal toxicity prediction of chemicals using TFS-PLS method in conjunction with active QSAR modeling, Abstracts of the 53rd Congress of the European Societies of Toxicology (EUROTOX) Bratislava, Slovakia, 10th–13th September, 2017. ; *Toxicology Letters* 280S (2017) S316.
- 5) 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, Tsuchiura, Nov., 2017.