Title of Research:

12_S04-01

Development of *in silico* Prediction Model on Environmental Fate of Chemical Substances

Principal Investigator:

Tatsuya Takagi, Graduate School of Pharmaceutical Sciences, Osaka University; Genome Information Research Center, Research Institute for Microbial Diseases, Osaka Univ.
1-6, Yamadaoka, Suita, Osaka, Japan, 565-0871, (tel) +81-6-6879-8243,
(e-mail) ttakagi@phs.osaka-u.ac.jp

Collaborators:

Norihito Kawashita, Graduate School of Pharmaceutical Sciences, Osaka University; Genome Information Research Center, Research Institute for Microbial Diseases, Osaka Univ.
1-6, Yamadaoka, Suita, Osaka, Japan, 565-0871, (tel) +81-6-6879-8244, (e-mail)
kawasita@gen-info.osaka-u.ac.jp
Kousuke Okamoto, Graduate School of Pharmaceutical Sciences, Osaka University;
1-6, Yamadaoka, Suita, Osaka, Japan, 565-0871, (tel) +81-6-6879-8242, (e-mail)
okamotok@phs.osaka-u.ac.jp

Summary of Research:

In 2009, since the Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc., was revised, chemical substances which are readily degradable have become subject to control under the law. Chemical industries are required to examine various physical, chemical, and biological properties of compounds such as toxicity, accumulation behavior, and degradation property. If there is a procedure which enables us to predict any properties of new or existing chemical substances without experiments, we are able to plan the efficient order of the experiments based on the ranking of the predicted properties. Because most existing prediction models on abiotic degradation, especially photolysis and hydrolysis are targeted to similar chemical substances, the development of the prediction models on the photolysis and hydrolysis of more various chemical substances would be contributed to obtain the effective ranking of candidates for experimentation.

The experimental results of the direct photolysis and hydrolysis under certain conditions were collected and then the datasets of hydrolysis and direct photolysis consisted of the results of 143 and 106 compounds, respectively. Although the experimental results of indirect photolysis were also checked, since there were few results whose experimental conditions were under the EPA guideline, we decided that the prediction on photolysis of this project was focused on direct one. We are intended to collect the information on photolysis and hydrolysis and to add it into the dataset continuously. The quantitative model on hydrolysis of “unstable” compounds whose half-lives are less than a year was built by using publicly available software, and its prediction performance was adequate. We are preparing to calculate an excited state that is regarded as a key factor for the prediction of direct photolysis of a compound using publicly available software. The trial system which provides the prediction models through the WWW was constructed. We are adding several functions and improving usability of this web site.

Timeline: November 1, 2012 –

Topics:

The 2th Annual Conference of New LRI, “Development of new tool for in silico prediction of environmental fate of compounds”, Aug 30, 2013

Publications:

The 40th Symposium of Structure-Activity Relationships, Aichi, Japan, Nov 2012