Title of Research:

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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.

In this term, the qualitative models for predicting whether a compound is stable to hydrolysis or not were developed. In our procedures for predicting hydrolysis, a predicted compound is classified to binary evaluation for hydrolysis by these qualitative models at first. If the compound is not stable to hydrolysis then its half-life is predicted by the quantitative models. and thus a sequence of our procedures for hydrolysis were completed. Additionally, availability domain in each prediction model was defined. The ground state and excitation states were calculated by DFT and TD-DFT in all compounds included in the dataset for predicting direct photolysis, and then five indices were calculated from excitation energies and oscillator strength of the excitation states. The plots between the index and the category based on half-life of the compounds suggested the correlation between the two variables and the area under the curve (AUC) values of the binary predictions of direct photolysis half-life based on the index were around 0.75. The web site for providing our prediction models of the hydrolysis was limitedly opened and the prototype of web site which provides the prediction models of the direct photolysis was constructed.

Timeline: Nov 1, 2013 - Feb 28, 2015

Topics:

The 3rd Annual Conference of New LRI, “Development of new tool for in silico prediction of environmental fate of compounds”, Aug 29, 2014

Publications:

5th FIP Pharmaceutical Sciences World Congress, Melbourne, Australia April 2014 (Oral session)
The 42th Symposium of Structure-Activity Relationships, Kumamoto, Japan, Nov 2014 (Oral session)