Title of Research:

Construction of prediction models for toxicities induced by drugs and chemicals based on chemical structures and AOP

Principal Investigator:

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Summary of Research:

QSAR models for activities of Adverse Outcome Pathways (AOPs) were constructed using machine learning methods. Moreover, a chemical structure-AOP-adverse effect database was constructed from the Tox21-AOP database and other adverse effect databases, such as JADER in Japan and FEARS in the USA. As a result of analyses of these integrated databases, random forest models indicated good prediction performance. Furthermore, it was showed that many kinds of adverse effects are related to AOP activities in the database.

Timeline:

March, 2016 – February, 2017

Topics:

Poster presentation, “Prediction for Activators of Adverse Outcome Pathways based on the Tox21 10K Compound Library”, ICCA-LRI and NIHS Workshop

Publications:

1. Yoshihiro Uesawa, "High-performance prediction of adverse outcome pathways based on machine learning methods with chemical structures", 31st JSSX Annual Meeting, symposium, invited lecture (invited), 2016/10/15
2. Yoshihiro Uesawa, "QSAR prediction of adverse outcome pathways based on machine learning methods", In-House Lecture, Sumitomo Chemical Company, Limited (invited), 2016/9/26
3. Yoshihiro Uesawa, "Construction of QSTR prediction models based on chemical structures"CBI Annual Meeting 2016, Focused session (invited), 2016/10/25
4. Yoshihiro Uesawa, "Analyses of chemical structures related to adverse outcomes based on large scale database", CBI Annual Meeting 2016, Focused session (invited), 2016/10/27
5. Yoshihiro Uesawa, "The Development of Highly Accurate Toxicity Prediction Methods Using the JMP® Machine Learning Function", Discovery Summit Japan, 2016/11/18
6. Jun Teraoka, Yurie Yoshida, Ryota Higuchi , Yuhei Mashiyama, Yoshihiro Uesawa, "Study of Effects of NF-κB for Reporting Frequency of Adverse Drug Reactions based on Tox21-AOP Database", CBI Annual Meeting 2016, 2016/11/27
7. Yuhei Mashiyama, Yurie Yoshida, Ryota Higuchi , Jun Teraoka, Yoshihiro Uesawa, "Analyses of Chemical Properties Associated with Reporting Frequency of Erythema Exudativum Multiforme Major in Adverse Drug Reaction Database", CBI Annual Meeting 2016, 2016/11/27
8. Ryota Higuchi, Yurie Yoshida, Jun Teraoka, Yuhei Mashiyama, Yoshihiro Uesawa, "Analyses of Chemical Properties Associated with Reporting Frequency of Interstitial Lung Disease in Adverse Drug Reaction Database", CBI Annual Meeting 2016, 2016/11/27
9. Yurie Yoshida, Ryota Higuchi, Jun Teraoka, Yuhei Mashiyama, Yoshihiro Uesawa, "Analyses of Chemical Properties for Reporting Frequency of Thrombocytopenia in Adverse Drug Reaction Database", CBI Annual Meeting 2016, 2016/11/27
10. Yoshihiro Uesawa, "Dragon descriptors develop computational toxicology"The seminar on the Dragon descriptors (invited), 2016/12/22