Title of Research:

16_PT01-02-3

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

Principal Investigator:

Yoshihiro Uesawa

Summary of Research:

Quantitative structure–activity relationship (QSAR) analysis applies structural and quantum chemical, and physicochemical features, calculated from molecular geometry as explanatory variables, to predict physiological activity. In current studies, the applications of QSAR prediction models in a variety of adverse effects such as Delirium, pulmonary edema, nausea/vomiting, respiratory depression, somnolence, rash, diarrhea, loss of appetite, nephritis, uterine cancer ... etc., have been constructed by databases such as JADER and FAERS (JAPIC-AERS). Furthermore, data set that includes FAERS and Tox21-AOP/MIE data was constructed and applied to analyze the relationship between adverse effects and major MIEs such as nuclear receptors and stress response pathways.

Timeline:

March 1, 2018 – February 28, 2019

Topics:

Uesawa, Y., inventor; Meiji Pharmaceutical University, assignee. Prediction systems, prediction methods, prediction programs, learning model input data generation systems, and learning model input data generation programs. Pending Japanese patent application 2018-122565（PTC）. 2018.

Matsuzaka, Y., Uesawa, Y.; Excellent Poster, CBI Annual Meeting 2018.

Asato, S, Kagaya, H., Uesawa, Y.; Excellent Presenter, The 4th Regulatory science forum for young people. 2018.

Publications:

1. Uesawa Y, "Quantitative structure-activity relationship analysis using deep learning based on a novel molecular image input technique", Bioorg Med Chem Lett, 28(20):3400-3403 (2018)
2. Matsuzaka Y, Uesawa Y, "Optimization of a Deep-Learning Method Based on the Classification of Images Generated by Parameterized Deep Snap, a Novel Molecular-Image-Input Technique for Quantitative Structure–Activity Relationship (QSAR) Analysis", Frontiers in Bioengineering and Biotechnology, in press (2019)
3. Ayano Shiota, Hajime Kagaya, Yoshihiro Uesawa, "Analysis of drug-induced somnolence based on JADER with chemical structure information", 138th annual meeting of the pharmaceutical society of Japan, Sendai Japan, 2018/3
4. Yuina Tatsuhiro, Hajime Kagaya, Yoshihiro Uesawa, "Analysis of structural and physicochemical features of drugs that cause non-cardiogenic pulmonary edema using Japanese Adverse Drug Event Report database (JADER)", 138th annual meeting of the pharmaceutical society of Japan, Sendai Japan, 2018/3
5. Yoshiyasu Ozu, Hajime Kagaya, Yoshihiro Uesawa, "Classification of constipation-related diseases using Japanese Adverse Drug Event Report database (JADER)", 138th annual meeting of the pharmaceutical society of Japan, Sendai Japan, 2018/3.
6. Sumino Asato, Hajime Kagaya, Yoshihiro Uesawa, "Construction of a prediction model for nausea and vomiting based on JADER with chemical structures", 138th annual meeting of the pharmaceutical society of Japan, Sendai Japan, 2018/3
7. Yuka Seta, Hajime Kagaya, Yoshihiro Uesawa, "The analysis on drug-induced delirium using Japanese Adverse Drug Event Report database with chemical structure information", 138th annual meeting of the pharmaceutical society of Japan, Sendai Japan, 2018/3