Waraporn Jungtanasombut 2012: Acute Toxicity Determination on Zebrafish Embryos and Octanol/Water Partition Coefficient of Azo Dyes: Experimental and Computational Investigations. Doctor of Philosophy (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Associate Professor Supa Hannongbua, Dr.rer.nat. 94 pages.

Based on EU legislation called REACH, it aims to manage chemicals and increase the protection of human health and environment from chemical used, manufactured and distributed within EU. Synthetic azo dyes that have been extensively used for textile dyeing should be one kind of the most synthetic dyes investigated their toxicity on aquatic organisms. This is because 2-50% of azo dyes can be lost to wastewater during dyeing process and ultimately relased to environment. Zebrafish embryos that is one kind of aquatic life and has been extensively used for toxicity determination because of their various advantages were utilized to investigate the acute toxicity (96 h) of 5 azo dyes including reactive red 239, direct red 80, direct blue 78, direct balck 22, and acid yellow 199 in this study. Endpoints were determined in this work including mortalitiy and embryo abnormalities. Results indicate that almost azo dyes in this study are nontoxic compound to zebrafish embryos due to their median lethal concentration (LC_{50}) is higher than 100 mg/L. However, industry using these dyes should be aware of their adverse effects because they can make developmental abnormalities on zebrafish embryos including yolk sac edema, cardiac edema, bent spine and tail malformation. In this study, acid yellow 199 is the highest toxic compound on zebrafish embryos due to its LC_{50} value is lowest. This results corresponsed to the experimental log P value derived from shake-flask method in this research. Acid yellow 199 has the highest log P value therefore, it tends to be easily absorbed in tissue of zebrafish embryos more than other compounds which have lower log P values. A QSTR model on the small set of 5 azo dyes built up by using linear regression method, it also supported that toxicity of compounds increases with increasing log P values. However, the quality of model is not good for toxicity prediction so, more toxicity data are required for developing a new QSTR model.

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