Waraporn Jungtanasombut 2008: Computational Toxicity in Substituted Benzene Derivatives for Dyes Production: A QSAR Investigation. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Associate Professor Supa Hannongbua, Dr.rer.nat. 56 pages.

Benzene derivatives are widely used for dyes production. Some of these compounds show a significant part of the chemicals that are of environmental concern and also to human health. Therefore, quantitative structure-activity relationship (QSAR) method has been applied to investigate the relationships between the structure and toxicity of substituted benzene derivative against *Tetrahymena pyriformis*, protozoa. Initial three dimensional molecular structures of chemicals were searched from SciFinder Database. All geometries were minimized and calculated for atomic charge by using SYBYL 7.0. Then structural descriptors of compounds were calculated by using MOE program. The best log (IGC^{-1}_{50}) model (the negative logarithm of 50 percent growth inhibitory concentration against *T. pyriformis*), which is satisfactory in both statistical significance and predictive ability, was derived from multiple linear regression (MLR). This model consists of three physical properties descriptors as the following: molecular weight (Mw), sum of the atomic polarizabilities (apol), and octanol-water partition coefficient (log P). The equation is log (IGC^{-1}_{50}) = -1.308(±0974) + 0.016(±0.003) Mw -0.053(±0.046) apol + 0.178(±0.190) log P, yielding statistics: r^2 = 0.773, s = 0.277, and F = 37.439. From obtained QSAR model showed that molecular bulk, molecular polarizability, and hydrophobicity of compounds are directly relate to toxicity. The major parameter affect to toxicity is log P that indicated the partitioning of each toxicant into biophase and may have a role in the toxicity.

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