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Theoretical Study on QSAR Analysis for Endocrine Disruptor

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Theoretical study for endocrine disruptors using QSAR (Quantitative Structure-Activity Relationship) analysis can provide an elegant approach to estimate their toxicity. We are aiming to build up a “Computer-Assisted Estimation System for Toxicity of Endocrine Disruptors”. We have improved the results of QSAR analysis by taking into account not only fragmentary information on ligand molecules but also the receptor-ligand interaction energies and physical/chemical properties for ligand. In order to estimate the toxicity more correctly it is effective to take in logP, Solubility and pKa of the compounds to QSAR analysis.

In this study, we have developed novel equations for estimation of logP, solubility, and pKa using Neural Networks. The method can be estimated easily and rapidly using only fragment based on group contribution method. The fitting result of total data set has high accuracy better than any other estimation method. The predictive capability of our method has been demonstrated on the result of test data set. The quality is sufficient for practical prediction of logP, solubility and pKa.