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QSAR Studies on Placental Transfer and Milk Excretion of Drugs - Clinical QSAR (2)

(Graduate School of Pharmaceutical Sciences, The University of Tokushima.) ○Yuki Hibino, Takashi Fujiwara, Shinichi Kobayashi, Masaru Kihara, Kumiko Sakamoto, Aiko Yamauchi, Hiroshi Chuman

When lactating mothers and pregnant women need to take medicines, it is very important to evaluate risk potential of drugs to their babies and fetus. However, there is little information about the drug excretion into human breast-milk and human placental drug transport.   In this study, we tried to analyze and predict the human M/P (milk to plasma drug concentration) ratio in and the human F/M (fetal to maternal drug concentration) ratio using various physicochemical characteristics of drugs. As the result of multiple regression analysis, the value of log M/P was computed to be dependent on the explanatory variables such as hydrophobicity (log P), molecular weight (log MW) and extent of ionization (log $[f^{un}(P) / f^{un}(M)]$) with a highly significant correlation coefficient. On the other, the value of log F/M was correlated with log MW and log P in drugs with low lipophilicity (log $P < 2$). Present results show that the QSAR methodology allows us to predict the drug excretion into milk and placental drug transport using the clinical data of human.