다중회귀 분석을 이용한 농약의 토양흡착계수
및 옥타놀/물 분배계수 예측
MULTIPLE REGRESSION ANALYSIS OF SOIL ADSORPTION COEFFICIENT
AND LOGP WITH VARIOUS MOLECULAR PROPERTIES

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Quantitative structure property relationships of soil adsorption coefficient (Koc) and various molecular properties of 89 pesticides were studied.

Octanol-water partition coefficients(LogPs) were estimated by HPLC with oc tadecyl column and compared with those of shake flask method.

From the statistical analysis, HPLC method could successfully predict logPs by shake flask method and the values were adopted for Koc estimation. Soil adsorption coefficients were also obtained from HPLC with cyanopropyl column.

From the multiple linear regression analysis, Koc from HPLC method showed good correlation with logP, water solubility and melting point. Because logP could be expressed with melting points and other molecular properties, predicti on equation could be summarised with logarithm of water solubility and melting point

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