

## Quantitative structure-property relationship (QSPR) study of n-octanol-water partition coefficients ( $\log P_{o/w}$ ) of fatty acids using multiple linear regression (MLR)

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**Abstract** The training set of 20 fatty acids with regularly distributed  $\log P_{o/w}$  values was used to assess the predictive ability of the QSPR/QSAR models produced in the regression. All the structures studied in this work were optimized by using B3LYP method in conjunction with 6-31G\* basis set. Statistical characteristics of the best model are the following:  $n = 20$ ,  $R^2 = 0.999$ ,  $R^2_{CV} = 0.997$ ,  $F = 2938$ , standard error (SE) = 0.148 and Durbin-Watson (DW) = 2.606

**Keywords:** QSPR, Partition coefficients ( $\log P_{o/w}$ ), Fatty acids, Multiple linear regression (MLR).

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