

quantitative structure-activity relationship (QSAR) (in drug design)

Quantitative structure-activity relationships (QSAR) are mathematical relationships linking chemical structure and pharmacological activity in a quantitative manner for a series of compounds. Methods which can be used in QSAR include various regression and pattern recognition techniques.

QSAR is often taken to be equivalent to *chemometrics* or multivariate statistical data analysis. It is sometimes used in a more limited sense as equivalent to Hansch analysis. QSAR is a subset of the more general term SPC.

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