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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.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1149

