Abstract

This paper proposes a new correlation index, named C, designed to measure the ability of a QSAR equation to correctly identify molecules characterized by high/low values of biochemical activity. Using observed/computed values of this activity - using examples taken from literature - we have compared the value of index C with the square of the Pearson $r^2$, Spearman $\rho^2$, and Kendall $\tau^2$ correlation indices. If $r^2$ is big ($r^2 > 0.7$) then the values of $r^2$, $\rho^2$, $\tau^2$ and C are quite well correlated, but if $r^2$ is low ($r^2 < 0.7$) then the correlation of $r^2$, $\rho^2$, $\tau^2$ and C is rather poor.

Author Keywords

Correlation indices; Descriptor correlation; QSAR

Matched Terms:

Chemicals and CAS Registry Numbers: calcium phosphate; berilium

See the Extended format page for all index keywords in this document.

References (10)


