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A correlation index for high and low value classes with applications to QSAR studies

Tarko, L.

Centre for Organic Chemistry, Romanian Academy, Bucharest, 202B Spl. Independenţei, 060023, Bucureşti, Romania

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 ρ^2, and Kendall τ^2 correlation indices. If r^2 is big ($r^2 > 0.7$) then the values of r^2, ρ^2, τ^2 and C are quite well correlated, but if r^2 is low ($r^2 < 0.7$) then the correlation of r^2, ρ^2, τ^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.

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Tarko, L.; Centre for Organic Chemistry, Romanian Academy, Bucharest, 202B Spl. Independenţei, 060023, Bucureşti, Romania; email:ltarko@cco.ro

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