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Qsar study on dipeptide ace inhibitors

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ABSTRACT. Quantitative Structure-Activity Relationships (QSARs) establish a mathematical relation between the biological activity of chemical compounds and their molecular structure. They provide quantitative models aimed to accurately predict a certain activity from the structural attributes. This topic has become a well-delimited branch in chemistry and was favored by the progress in computer science. Cluj property indices are used for modeling the ACE inhibition biological activity of a set of 58 dipeptides, taken from the literature. Description of dipeptide molecules is made by using the fragmental property Cluj indices. Four models were taken into consideration: two of them topological (dense topological and rare topological) and two others geometric (dense geometric and rare geometric). In these models, a weak dependence on distance for the potential function (gravitational and Coulombian), in uniform field, and a strong dependence on distance for the potential, that generates a non-uniform field, were considered. The indices are calculated as local descriptors of some fragments of the molecule and, a global index is then obtained by summing the fragmental contributions. The statistics were performed by STATISTICA software package. The results are compared to those reported in some previous works.

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