Counter propagation artificial neural networks modeling of an enantioselectivity of artificial metalloenzymes.

Autorzy

Sylwester Mazurek

T. R. Ward

M. Novič

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Streszczenie

The counter propagation artificial neural networks (CP-ANNs) were used to develop a quantitative structure-selectivity relationship (QSSR) for a set of artificial metalloenzymes. The artificial metalloenzymes consist of biotinylated rhodium-diphosphine complexes incorporated in streptavidin mutants acting as host protein. Such hybrid catalysts have been shown to be good enantioselective hydrogenation catalysts for acetamidoacrylic acid. The descriptor-based models were constructed to predict enantiomeric excess (%ee) on the basis of the catalyst structures originating from docking simulations. 3D molecular descriptors for the docked ligands structures were computed. The relative arrangement of guest and host molecules was coded using distance descriptors (Rh-C(alpha) interatomic distances); the diversity of the mutant proteins at the position S112 was coded with molecular descriptors for the sequence of three neighboring amino acids (T111-S112X-G113). The selection of testing samples for the external model validation was based on the Kohonen mapping. The final model trained by two thirds of the entire dataset was characterized by satisfactory statistical parameters for the external test set (R = 0.953 and RMS = 16.8 %ee). The proposed procedure of docking-based descriptor generation thus appears as a promising alternative to the full characterization of the complex structure by experimental or computational methods.

Adres publiczny

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http://link.springer.com