Modeling the Relationship between Biological Activity of Delta-selective Enkephalin Analogues and Docking Results by Polynomials

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One of the areas of bioinformatics is to develop a fast and reliable method for predicting the biological activity of compounds. This will facilitate the design of new compounds and reduce costs. The process of creating the selective ligands of delta opioid receptor (DOR) was directed towards the synthesis of enkephalin analogues. Their biological activity was determined using the *in vivo* and *in vitro* methods, allowing establishing the relationship between structure and biological activity. The relationship of the efficacy with the values of the so-called ChemScore scoring function from GOLD 5.2 and the values of total energy of ligand-receptor complex was modeled with first- to third-degree polynomials and surface fitted method. The polynomial surface of the third degree has the best fit, assessed by least squares method. In our previous study with the theoretical model of DOR (PDBid:1ozc) it was established the relationship of the efficacy with the values of the GoldScore scoring function and the values of total energy of ligand-receptor complex. This relationship was modeled with third degree of polynomial in Matlab. The GoldScore scoring function is used for the prediction of ligand binding positions. In contrast to it the Chemscore scoring function takes account of hydrophobic-hydrophobic contact area, hydrogen bonding, ligand flexibility and metal interaction. The aim of presented work is to find an optimal fitting polynomial function by which to model the relationship between quantitative parameters of *in vitro* bioassay and the values obtained from docking with crystal structure of DOR (PDBid:4ej4). The third degree polynomial is successfully used for modeling of the relationship between the efficacy of delta-selective enkephalin analogues and docking results.

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