Comparative Evolution of four Scoring Functions with three models of Delta Opioid Receptor using Molecular Docking

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The present study was performed in order to find the most appropriate scoring functions and the model for docking of enkephalin analogues with delta-opioid receptor (DOR) that correlated well with the results obtained from *in vitro* tests.

The capabilities of the four scoring functions embedded in GOLD were explored with three different models of DOR: a theoretical model published in ePDB (id: 1ozc), a model obtained by as with homology modeling, and a crystal structure of DOR published in PDB (id: 4ej4). Eleven enkephalin analogues were consistently docked with each of the models with each of the four scoring function.

The analysis of the obtained results shows that after the docking with our modeled DOR values of scoring functions correlate with the data from *in vitro* tests at the highest degree. Furthermore, the use of the scoring functions ASP (Astex Statistical Potential) and GoldScore enable more precise docking of the test ligands as correlation coefficients were: ASP score/ IC_{50}=−0.86, ASP score/K_A = −0.94, and GoldScore Fitness/e_{rel}=−0.66, respectively.

Hence, for the design of new selective and active analogues of enkephalins our model of DOR with the application of ASP function should be used.