Quantitative Analysis and Mathematical Models of a Partial Agonism

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The purpose of this research paper is to show the results of a study on Quantitative Structure-Activity Relationships (QSAR), mathematical and computer models for determination of the relation between the structure of the compounds and the induced by them measurable biological effect.
The key points of the research paper are: 1) Binding Mechanisms, 2) Docking Problem, 3) Models of partial agonism, 4) Parameters characterizing the partial agonism. The theoretical models and results presented for each of the key points are supported by experimental data obtained by studies of mu- and delta- opioid ligands for mu- and delta- opioid receptors [1].
The new results from this research are: (a) Applying the Castillo-Katz scheme for ligand-receptor interactions; (b) The properties of the ligands, obtained *in vitro* experiments, have been confirmed through molecular docking of mu- and delta- opioid receptors with mu- and delta- opioid ligands [2,3]; (c) A generalization of the Theoretical Hyperbolic Model [4] about the partial agonism, through applying the Castillo-Katz scheme; (d) Explicit formulas for affinity and Stephenson's efficacy of partial agonists.

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