Ph.D. projects in progress

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Doctoral school: Faculty of Medicine, University of Szeged, Theoretical Medicine Doctoral School

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Title of the research topic: Modelling ligand characteristics and receptor specificity in the opioid system

Description of the research topic: The opioid system plays an inevitable role in the medication due to its involvement in the antinociception. It includes four receptor types. This complex system affects numerous physiological processes resulting in a difficult balance between the desired and side effects. Understanding the molecular background of the different pharmacological effects (agonism, antagonism, inverse- and partial agonism) makes possible the improvement of this balance. The molecular background will be explored by in silico methods. Patterns of the interacting receptor atoms and the binding energies will be constructed to explain the different pharmacological features. The interaction patterns will be constructed by the existing experimental receptor structures and theoretical models for each opioid receptor.