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Ionotropic GABA receptors: modelling and design of selective ligands

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Ionotropic GABA_A and GABA_C receptors play an important role in the operation of CNS and serve as targets for many neuroactive drugs. Using the homology modelling and molecular dynamics, the 3D models of the receptors were built and some aspects of ligand-target interactions were elucidated [1,2].

To better understand the structural factors controlling the activity and selectivity of the ligands, a series of QSAR models [3] were derived based on the Molecular Field Topology Analysis (MFTA) [4], CoMFA and Topomer CoMFA approaches. They were compared with each other as well as with the molecular modelling results.

Finally, a number of potential selective ligand structures were identified by means of the virtual screening [5] from the available chemicals databases and the generated structure libraries.

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