Journal of Cheminformatics

POSTER PRESENTATION Open Access

# Ionotropic GABA receptors: modelling and design of selective ligands

Vladimir A Palyulin*, EV Radchenko, DE Osolodkin, VI Chupakhin, NS Zefirov

*From* 5th German Conference on Cheminformatics: 23. CIC-Workshop
Goslar, Germany. 8-10 November 2009

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.

Published: 4 May 2010

**References**

1. Osolodkin DI, Chupakhin VI, Palyulin VA, Zefirov NS: *J Mol Graph Model* 2009, **27**:813.
2. Chupakhin VI, Palyulin VA, Zefirov NS: *Doklady Biochem Biophys* 2006, **408**:169.
3. Chupakhin VI, Bobrov SV, Radchenko EV, Palyulin VA, Zefirov NS: *Doklady Chemistry* 2008, **422**:227.
4. Palyulin VA, Radchenko EV, Zefirov NS: *J Chem Inf Comp Sci* 2000, **40**:659.
5. Radchenko EV, Palyulin VA, Zefirov NS: *Chemoinformatics Approaches to Virtual Screening* RSCVarnek A, Tropsha A 2008, 150-181.

doi:10.1186/1758-2946-2-S1-P49
**Cite this article as:** Palyulin *et al.*: Ionotropic GABA receptors: modelling and design of selective ligands. *Journal of Cheminformatics* 2010 **2**(Suppl 1):P49.

Department of Chemistry, Moscow State University, Moscow 119991, Russia