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# A new conceptual understanding of the structure and function GABA-benzodiazepine receptor complex on the basis of the investigation of the molecular geometry and quantum-chemical characteristics main group anticonvulsants, inhibitor amino acids, and some convulsive agent

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**Statement of the Problem:** Until these days, searching of endogen agonists of benzodiazepine receptors is an actual task, because a lot of problems clinical medicine (in first turn neurology, epileptology, narcology deepened of understanding mechanism action and function GABA-benzodiazepine receptor complex to elaborate new perspective anticonvulsive and nootropic compounds.

**Purpose:** Investigate quantum mechanics characteristics and molecular geometry has three conformational states GABA: linear (GABA-1 conformer), bucket-like (GABA-3 conformer) agonists of which is bucket-like conformer of GABA and isoguvacine, but antagonists are picrotoxin and bicuculline; cyclic (GABA-2 conformer) agonists of which are cyclic conformer of GABA, glycine, and β-alanine, but antagonists are bemegride, pentylenetetrazol and strychnine; and GABA-3 receptors; Maine anticonvulsant's groups. Investigate nootropic's and anticonvulsants effects one-valence salts of glycine and GABA.

**Method:** The molecular geometry of the benzodiazepine's pharmacophores, main GABA conformers, and glycine were studied in the approximation of molecular mechanics with the use of the MM2 force field. Influence intraperitoneal injection different one-valence salts of glycine and GABA on the cerebral neurophysiological activity in white rats (taking of EEG) and their anticonvulsant activity using strychnine, picrotoxin, pentylenetetrazol, and maximal electro seizure models.

**Results:** It was shown, that anticonvulsive and other behavioral effects of derivatives of barbituric acid, benzazepine, benzodiazepine, gidantoine, succinimide, and oxazolidinone are realized probably via GABA-2 receptors to switch on them the following functional centers of their structure are necessary: α, and [δ-ε] for barbiturates; β, [δ-ε] and γ for carbamazepine; β and [δ-ε] for benzodiazepine derivatives, gabapentin and vigabatrin; α, β, γ and [δ-ε] for gidantoine and oxazolidinone derivatives; α, β, γ for succinimide derivatives. The expression of any (including nootropic) behavioral effects of anticonvulsants and inhibitory amino acids depends on power, location, and numbers of hydrogen bonds developed between active centers of pharmacophore of anticonvulsant or inhibitory amino acids and active centers of the functional skeleton of the GABA-2 receptor complex.

**Conclusion:** (1) The more stronger the charge on the atoms of the pharmacophore of the GABA agonist, the more expressive its anticonvulsant effect and vice versa, the weaker the charge on the atoms, the more expressive the nootropic effects appear (2) There are perspectives of synthesis of compounds, pharmacophore of which should be like as cyclic conformer of GABA, glycine, and β-alanine on their quantum mechanics characteristics and molecular geometry.

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