عنوان مقاله:

Molecular Modeling of the antagonist compound esketamine and its molecular docking study with non-competitive N-methyl-D-aspartate (NMDA) receptors NR1, NR2A, NR2B and NR2D

محل انتشار:

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نویسندگان:

Mehdi Nabati - *Synthesis and Molecular Simulation Laboratory, Chemistry Department, Pars Isotope Company, P.O. Box: ۱۴۳۷۶۶۳۱۸۱, Tehran, Iran*

Vida Bodaghi-Namileh - *Synthesis and Molecular Simulation Laboratory, Chemistry Department, Pars Isotope Company, P.O. Box: ۱۴۳۷۶۶۳۱۸۱, Tehran, Iran*

Saman Sarshar - *Physics Department, Faculty of Science, Lorestan University, Khorramabad, Iran*

خلاصه مقاله:

The main purpose of the present article is reactivity and stability properties study of the antagonist compound esketamine and analyzing of its binding to the non-competitive N-methyl-D-aspartate receptor subunits (NR1, NR2A, NR2B and NR2D). In first step, the molecular structure of esketamine was optimized using density functional theory (DFT) method at B3YP/6-311++G(d,p) level of theory. The reactivity and stability properties of the title medicinal compound were studied by global reactivity indices. The computational data showed the molecule is stable and has low tendency to interact with residues of the biomolecules like receptors and proteins. Secondly, the molecule binding to the receptors were analyzed by molegro virtual docker (MVD) program. Our computations indicated that the compound asserts its pharmacological effects mainly through interactions with NR2B receptors and the NR2B residues containing Gly [A] 128, His [A] 127, Gly [A] 264, Tyr [A] 282, Ser [A] 131, Asp [A] 265, Ser [A] 260 and Met [A] 132 are the main amino acids involved in the ligand-receptor complex formation.

کلمات کلیدی:

Esketamine, Major depressive disorder, Molecular docking, Molecular Simulation, N-methyl-D-aspartate receptor, Treatment-resistant depression