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QSAR, ADMET in silico Pharmacokinetics, molecular docking and molecular dynamics studies of novel bicyclo (aryl methyl) benzamides as Potent GlyT1 inhibitors for the treatment of Schizophrenia

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Forty-four bicyclo ((aryl) methyl) benzamides, acting as glycine transporter type 1 (GlyT1) inhibitors, are developed using molecular modeling techniques. QSAR models generated by multiple linear and non-linear regressions affirm that the biological inhibitory activity against the schizophrenia disease, is strongly and significantly correlated with physicochemical, geometrical and topological descriptors, in particular: Hydrogen bond donor, polarizability, surface tension, stretch and torsion energies and topological diameter. According to in silico ADMET properties, the most active ligands (L6, L9, L30, L31 and L37) are the molecules having the highest probability to penetrate the central nervous system (CNS), but the molecule 32 has the highest probability of being absorbed by the gastrointestinal tract. Molecular docking results indicate that Tyr124, Phe43, Phe325, Asp46, Phe319 and Val120 amino acids, are the active sites of the dopamine transporter (DAT) membrane protein, in which the most active ligands can inhibit the glycine transporter type 1 (GlyT1). The results of molecular dynamics (MD) simulation revealed that all five inhibitors remained stable in the active sites of the DAT protein during 100 ns, demonstrating their promising role as candidate drugs for the treatment of schizophrenia.

Recent Publications

1. Pharmaceuticals 2022, 15(6), 670; https://doi.org/10.3390/ph15060670
2. QSAR, ADMET In silico Pharmacokinetics, Molecular Docking and Molecular Dynamics Studies of Novel Bicyclo (aryl methyl) benzamides as Potent GlyT1 Inhibitors for the Treatment of Schizophrenia"Processes 2022, 10, 1462.
3. 3D-QSAR, ADME-Tox In Silico Prediction and Molecular Docking Studies for Modeling the Analgesic Activity against Neuropathic Pain of Novel NR2B-Selective NMDA Receptor Antagonists »
4. "QSAR, ADME-Tox, molecular docking and molecular dynamics simulations of novel selective glycine transporter type 1 inhibitors with memory enhancing properties"

Biography

Mohamed El fadili is a PhD student, chemistry sciences in USMBA university. He received certificate of participation in oral and technical presentation, recognition and appreciation of research contributions to 6th INTERNATIONAL EDUCATION AND INNOVATIVE SCIENCES CONGRESS. held on November 24-25, 2022 / Burdur Mehmet Akif Ersoy University, Türkiye and Certificate of participation in the 6th International Conference on Materials and Environment: 'ICME 6-2022' on December 19-20, 2022. This conference is organized by the Laboratory of Chemistry-Biology Applied to the Environment "LCBAE, URL-CNRST N°13, in collaboration with the Moroccan Association of Catalysis and Environment "AMCE"

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