عنوان مقاله:

In-silico screening, molecular docking, pharmacokinetics studies and design of histone deacetylase inhibitors as anti-Alzheimer agents

محل انتشار:

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نویسندگان:

.ABDULJELIL Ajala - *No I.۳ Galadimawa Street, Kakuri, Kduna State, Nigeria*

Adamu Uzairu - *Chemistry, Physical Sciences, Ahmadu Bello University, Zaria*

Gideon Shallangwa - *Department of Chemistry, Ahmadu Bello University*

Stephen Abechi - *Chemistry, Physical Sciences, Ahmadu Bello University, Zaria Nigeria*

خلاصه مقاله:

Alzheimer's Disease (AD) is a complex illness mechanism and an untreatable ailment that presently brings huge sorrow to patients and their relatives. Presently, the cure for this disease is zero. The existing drugs have several side effects. Therapeutic Chemistry, a vital field of research, has been working tirelessly to develop new treatments that can be effective in curing this disease. Design, molecular docking, and pharmacokinetic assessment (ADMET) methods are used to determine and confirm the sturdy configuration of the receptor pocket. ۱۶ Histone Deacetylase inhibitors have been docked with the acetylcholinesterase target for protein-ligand interaction. Compound ۲ was found to possess the highest binding scores of ۱۹.۷۵۸ kcal/mol. This was used as a template to design several HDAC derivatives, but seven of the designed compounds had higher binding scores and better interaction than the template; ۱:-۲۰.۰۳۱ kcal/mol, ۲:-۲۰.۵۸۳ kcal/mol, ۳:-۱۹.۹۲۵ kcal/mol, ۴:-۲۱.۶۳۹ kcal/mol, ۵:-۲۱.۹۵۰ kcal/mol, ۶:-۱۹.۹۱۷ kcal/mol, and ۷:-۲۳.۲۸۹ kcal/mol. The pharmacokinetics evaluation of these designed compounds (ADMET) results showed good drug-likeness and oral bioavailability scores. Based on the binding affinity scores of the designed compounds against AD, the designed compounds have superior pharmacological characteristics and can be used as neuro-therapeutic .candidates after rigorous in-silico investigation

کلمات کلیدی:

Alzheimer' s disease, Design, Drug-likeness, binding scores, multitarget-directed ligands