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Computational study of the anticholinesterase activities and selectivity of phenserine and its analogue hexserine

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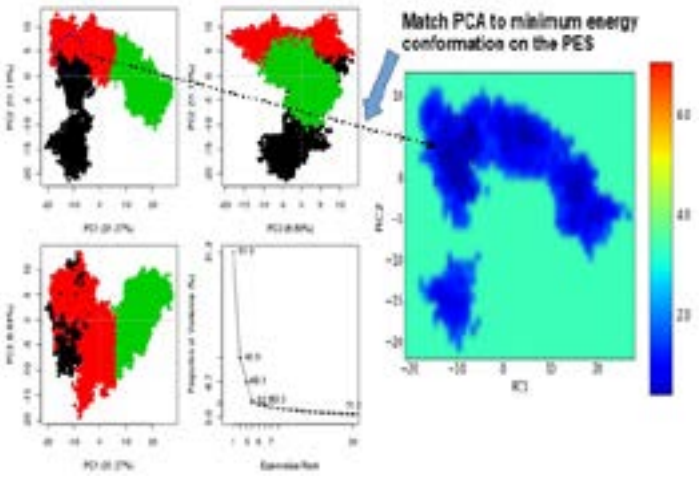
The common cause of dementia among the elderly is known to be Alzheimer's disease (AD) which is a disorder that results into a decline in progressive cognition and loss of memory due to the degeneration of the central nervous system. The compound HEX has been reported to show strong inhibitory activities against AChE than PHE and a very high selectivity for enzyme AChE over the enzyme BChE when compare to PHE (174-fold). The interest of this study is therefore use for classical molecular dynamic methods (CMD) and accelerated molecular dynamics (AMD) to give further insight into the selectivity of the HEX than PHE in their interaction with both AChE and BchE. High similarity in the RMSD of the two ligands with both AChE and BChE during the CMD and AMD trajectory were observed. Towards the end of the 20ns simulation of the AMD trajectory, the ligand HER seams to imposed new conformational change that resulted into its higher RMSD compare to the ligand PHR in both their interaction with AChE and BChE. As expected, a higher value of the RMSD was recorded for the AMD trajectory compare to CMD which is an indication of a greater number of conformational changes in the protein during the AMD. Our results show that the possible factors that contributes to the lower binding energy of PHE compare to HER especially in their interaction with AChE is as a result of penalizing effects of the generalized born solvent (ΔE_{egb}), poisson boltzmann solvent (ΔE_{epb}) and free energy of solvation (ΔG_{solv}).



Biography

Adebayo A. Adeniyi is currently a postdoctoral fellow from the University of the Free State, South Africa and is also an academic lecturer at the University of Oye-Ekiti, Nigeria. He got his PhD in chemistry at University of Fort Hare, South Africa in 2014. He specializes in physical and computational chemistry but have a broad knowledge of all area of chemistry. His research interest is to combine both computational and experimental methods for the design of novel molecules for therapeutic application in order to circumvent the present limitations like drug resistance, mutation and adverse side effects in chemotherapy. He has published more than thirty research articles in pear review journals. He is a Nigerian citizen and a Christian by religion. He is married to Joy N. Adeniyi and is blessed with handsome boy called Daniel A.I. Adeniyi.

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