Docking studies of drugs acting on Myasthenia Gravis

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In the present study and evaluation of commercially available drugs acting as inhibitors of specific enzymes used to reduce the symptoms of Myasthenia Gravis was performed in order to evaluate their interaction and consequently their action with target protein molecules. Myasthenia Gravis is a chronic autoimmune disease for the treatment of which mainly drugs targeting acetylcholinesterase are administered. Computational chemistry programs based on Molecular Binding were used in the preparation of this thesis to evaluate the binding of pyridostigmine, azathioprine and prednisone to target proteins. Specifically, the binding of molecules in twelve classes of enzymes to a binding site of each enzyme was studied: Human acetylcholinesterase (4EY7), Human butyrylcholisterase (5DYW), Human adenosine A1 (5UEN), Cathepsin K (1YK8), Carbonic anhydrase (4XIX) , Dehydrogenase (3D4N), Thimidine kinase (4UXJ), Cannabinoid CB1 (5XR8), Sars-Cov-2 (6LU7), Alkaline phosphatase (1ALK), Carbonic anhydrase XII (1JD0), Carbonic anhydrase VII (6H37). Using two computer programs, the types of bonds developed during the interaction of the binding molecules with the protein of each receptor were visualized. Studies on the stability and molecular interactions developed during protein-binding interaction, Molecular Dynamics simulations on the compounds that gave the strongest bindings and spectroscopic studies to verify the validity of the results were performed.

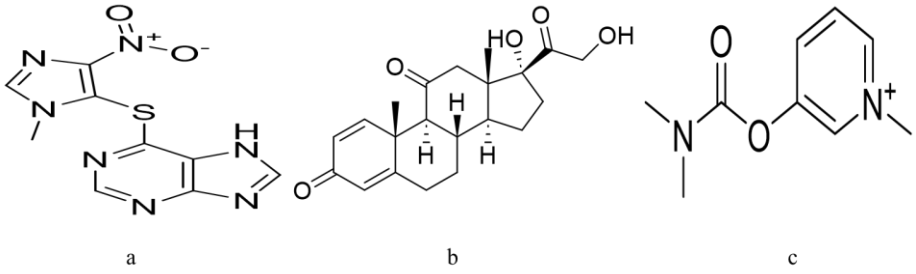

Figure 1: The chemical structure of Azathioprine (a), Prednisone (b) and Pyridostigmine (c).

References:

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