

**STUDY OF THE COMBINED EFFECT OF DEOXYPEGANINE AND
GALANTAMINE ALKALOIDS ON THE ACETYLCHOLINESTERASE
ENZYME BY DOUBLE DOCKING METHOD**

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It is known, in silico methods, particularly dual docking approaches, can serve as valuable tools for identifying complementary compounds suitable for co-administration with existing drugs or for the development of combination therapies [1].

In this regard, the interactions of galantamine (G), deoxypeganine (DOP), L-ascorbic acid (LAA) and D-ascorbic acid (DAA), as well as the binary compounds G-DOP, G-LAA, G-DAA, DOP-LAA and DOP-DAA with acetylcholinesterase (AChE, PDB ID: 4M0E) were investigated using both single- and double-ligand molecular docking approaches [3, 4].

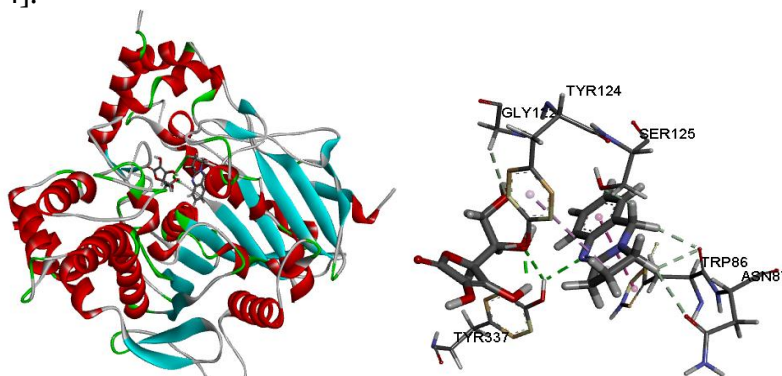


Figure 1. The docked AChE-DOP-DAA complex and interactions of ligands with amino acid residues

The double-docking results revealed that galantamine does not penetrate the active site of AChE. In contrast, deoxypeganine was able to access the active site and interact with key amino acid residues regardless of whether the accompanying ligand was L- or D-ascorbic acid or galantamine. Furthermore, in the G–LAA complex, L-ascorbic acid penetrated deeper into the active site and formed interactions with Ser203, a crucial residue of the catalytic triad. These findings suggest that deoxypeganine exhibits a stronger propensity for active-site binding than galantamine in dual-ligand docking systems.

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References:

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