MOLECULAR DOCKING CONTRIBUTION TO THE STUDY OF INTERACTIONS INVOLVING TRI²PEPTIDES WITH RESPECT TO ENZYMATIC TARGETS INCRIMINATED IN NEURODEGENERATIVE DISEASES

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Abstract - Neurodegenerative pathologies are considered as a public health problem, they constitute a handicap for the patients and their entourage especially in the advanced stages of the neurological attacks.Given the complexity and the multitude of physiopathological mechanisms implicated in neurodegenerative diseases, several research teams are currently undertaking as research projects, the evaluation of new proteins as therapeutic targets such as the family of protein kinases considered for a long time by the pharmaceutical industry as not druggable. Recently,It has been shown in several studies that molecules bearing peptic sequences are of interest in the treatment of certain neurodegenerative diseases such as the peptidic inhibitors of amyloid aggregation incriminated in Alzheimer's disease.
In this work, we were interested in the importance that three small tri peptide molecules (PFF, LVF, LVP) can bring in the inhibition of seven enzymes implicated in neurodegenerative diseases. A study by molecular Docking was carried out, the enzymes in question were: β secretase, γ secretase, Acetyl choline esterase, Mono Amino Oxidase, Map kinase p38, GSK3B and JNK. Our calculations were made using the MOE program (Molecular Operating Environment).
The obtained molecular docking results were interesting for the LVP-JNK and LVF-γ secretaseinteraction.

Key words - Alzheimer, Parkinson, molecular docking, Tripeptide, LVP, LVF, PFF, β secretase, γsecretase, p38 Map kinase, GSK3B, JNK, Acetyl choline esterase, MOAB.