

# THE POTENTIAL OF LOW-DOSE HYDROGEN PEROXIDE (H<sub>2</sub>O<sub>2</sub>) AS PREVENTIVE STRATEGI TO PARKINSON DISEASE

Athiyah Layla<sup>1</sup>, Sri Widyarti<sup>2</sup>, and Sutiman Bambang Sumitro<sup>2\*</sup>

<sup>1</sup>Master Program of Biology Department, Faculty of Mathematics and Natural Sciences, University of Brawijaya, Malang, Indonesia

<sup>2</sup>Biology Department, Faculty of Mathematics and Natural Sciences, University of Brawijaya, Malang, Indonesia

\*Corresponding author: [sutiman@ub.ac.id](mailto:sutiman@ub.ac.id)

## Abstract

The number of people with Parkinson's Disease (PD) is increasing every year in Indonesia. Some researchers stated that PD cannot be cured completely and it is not yet known how to prevent it. This is because the medical sector is still focusing on treating the symptoms of PD, and has not focused on preventing PD. PD is caused by the presence of  $\alpha$ -synuclein ( $\alpha$ syn) fibrils. Under normal circumstances  $\alpha$ syn is in monomeric form and unfolding. However, in patients with PD,  $\alpha$ syn misfolds and aggregates into amyloid fibrils that accumulate intracellularly.  $\alpha$ syn that forms fibrils becomes more toxic and cause the death of dopaminergic cells, which are dopamine-producing cells. Therefore, ideally a new treatment strategy should be developed, with complementary therapy using low-dose H<sub>2</sub>O<sub>2</sub> which has neuroprotective potential to prevent the formation of  $\alpha$ syn fibrils. This study was conducted in silico, starting with data collection: for H<sub>2</sub>O<sub>2</sub> molecules from Pubchem,  $\alpha$ syn from protein data bank (PDB). Furthermore, H<sub>2</sub>O<sub>2</sub> docking with  $\alpha$ syn protein was carried out using PyRx 0.9.8. For docking between  $\alpha$ syn monomers using HDOCK online software. Followed by molecular dynamic simulation using YASARA. The results of molecular docking showed that H<sub>2</sub>O<sub>2</sub> reduce the binding affinity of fellow  $\alpha$ syn monomers and also affect the active site, causing changes in interactions. The results of molecular dynamics showed that

the presence of  $\text{H}_2\text{O}_2$  causes  $\alpha\text{syn}$  to unfold and increase fluctuations in active site residues, which allows for the release of bonds between  $\alpha\text{syn}$  monomers. Thus, it can be concluded that the  $\text{H}_2\text{O}_2$  molecule has the potential to prevent the formation of  $\alpha\text{syn}$  fibrils, and has potential as a preventive treatment in PD.

*Keywords:  $\alpha\text{syn}$  fibrils, hydrogen peroxide, parkinson's disease, preventive strategi.*