## IJARSCT



International Journal of Advanced Research in Science, Communication and Technology

International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal

Volume 5, Issue 6, May 2025



## In Silico Studies on Neuroprotective Effects of Moringa Oleifera With Molecular Docking.

Mr. Sidharth Rajendra Wade<sup>1</sup>, Mr. Niraj Rajendra Wadile<sup>2</sup>, Ms. Rutuja Raosaheb Waghmode<sup>3</sup>, Mr. Manoj Vijay Wavare<sup>4</sup>, Mr. Arunkumar Umeshchandra Yadav<sup>5</sup>, Ms. Harshali Thakare<sup>6</sup>, Mr. Abhishek Kumar Sen<sup>7</sup>, Principal Prof. (Dr.) Sonali Vinod Uppalwar<sup>8</sup>. Ideal Institute of Pharmacy, Posheri, Wada.

Abstract: Progressive loss and destruction to neurons is a hallmark of neurodegenerative diseases, which include Parkinson's and Alzheimer's. Historically, a variety of illnesses have been treated with Moringa oleifera, a plant with a wide range of therapeutic uses. Through the use of in silico techniques, this study sought to examine the possible therapeutic effects of Moringa oleifera components on neurological illnesses. In order to find possible lead drugs that target important proteins linked to neurodegenerative disorders, molecular docking and virtual screening were used. Our findings demonstrated that a number of Moringa oleifera compounds have positive interactions and high binding affinities with target proteins, indicating their potential as medicinal agents. The stability and binding free energy of these compounds were further confirmed by molecular dynamics modeling. This study shows that Moringa oleifera compounds have the potential to be effective treatments for neurological illnesses and sheds light on the molecular mechanisms behind their therapeutic benefits.

**Keywords**: Moringa oleifera, neurodegenerative diseases, in silico studies, molecular docking, virtual screening, molecular dynamics simulation



