Green Synthesis of Cerium Oxide Nanoparticles Supported by Molecular Docking–Driven Identification of Bioactive Phytocompounds from *Cymodocea serrulata*

Sethu Meenal[1], Halliah Gurumallesh Prabu[1], Thambusamy Stalin[1], Mahalingam Sundhararajan[1], Jeyaraman Jeyakanthan[2]

[1]Department of Industrial Chemistry Alagappa University, Karaikudi, Tamil Nadu, India

[2]Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India

Corresponding author Email: hgprabhu@alagappauniversity.ac.in

Abstract

The *Cymodoceaceae* family of seagrasses, which *includes Cymodocea serrulata, Amphibolis, Halodule, Syringodium*, and *Thalassodendron* was investigated for phytocompounds compounds in this work that might stabilize and reduce the cerium ions for green synthesis of cerium oxide nanoparticles (CeONPs). *Cymodocea serrulata* was selected for its rich phytocompounds based on GC-MS analysis. Form this analysis, a number of 112 phytocompounds were found and molecular docking was performed. According to the results, the top three were found using the highest docking score. Additionally, the *Cymodocea serrulata* extract was used to synthesis CeONPs using the Soxhlet method, and XRD, FT-IR, and UV-Vis spectroscopy were used to characterize them. The synthesis of CeONP was indicated by the UV-Vis spectra significant absorption at 320 nm. FT-IR result revealed shifts in functional group vibrations, confirming phytochemical involvement in CeONP synthesis. XRD confirmed the crystalline nature and size distribution of CeONPs. Based on the in silico and synthesis results, the designed CeO NPs may be suitable for further advanced characterization and in vitro studies for the development of an effective drug-delivery vehicle.

Keywords: *Cymodocea serrulataI,* CeONPs*, In silicoI*, Phytocompounds, Seagrasses.