Computational and Experimental Investigation of phytocompounds from *Andrographis echioides* plant and synthesis of Metal Oxide nanoparticles by green method

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Abstract

Green synthesis of metal nanoparticles plays a vital role in producing the tiny particles along with the desired morphology. It is an effortless, affordable, and environmentally friendly substitute for conventional chemical and physical synthesis techniques. This study focuses on plant-mediated metal oxide nanoparticles for biomedical applications. The Indian medicinal plant *Andrographis echioides* has been selected, possessing various phytocompounds that produce the specified nanoparticle size due to having reducing and stabilizing agents. An aqueous extract of *Andrographis echioides* was prepared by the decoction method and characterized by GC-MS techniques to identify the phytocompounds. Cerium oxide nanoparticles were synthesized using *Andrographis echioides* by the simple stirrer method. Both samples, such as extract and Cerium Oxide nanoparticles were physically characterized by different techniques such as UV-Vis, FT-IR, XRD, and TEM analysis. Following this, the identified phytocompounds were used to perform *in silico* approaches, including Molecular Docking, ADME prediction, and Molecular Dynamics Simulation studies. All the physical study revealed that the formation of Cerium Oxide nanoparticles has been successfully synthesized. The In silico study showed that the top three phytocompounds are selected for further therapeutic development based on the higher Docking score, number of molecular interactions, drug likeness and pharmacokinetic properties.

Keywords: *Andrographis echioides,* anticancer activity, Cerium oxide nanoparticles Characterization Techniques, *In silico* study, Phytocompounds.