Structural analysis, molecular dynamics and docking calculations of skin protective tripeptide and design, characterization, cytotoxicity studies of its PLGA nanoparticles.

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The main purpose of current study is to analyze the structural behaviour of a skin protective tripeptide Gly-His-Lys (GHK) with anti-oxidant and anti-cancer properties, design and characterize its nanoformulation by experimental and spectroscopic techniques to ensure its stability and enhance bioavailability and biocompatibility.

GHK is extensively used as a cosmetic products for the therapy of skin and hair deformation. In this study the calculations on GHK were performed at DFT/B3LYP level of theory with the 6–311++G (d,p) basis set to obtain optimized geometry, HOMO-LUMO energy gap, MEP analysis and vibrational wavenumbers.

The spectroscopic investigation of GHK tripeptide was performed experimentally through optical spectroscopic techniques (such as FT-IR, FT-IR-ATR and Micro-RAMAN) and compared with theoretical wavenumbers. The Potantial Energy Distributions (PED) of the normal modes of vibrations were also carried out with the help of GAR2PED program. By using molecular dynamics simulation, the stability of the GHK in water and methanol mediums have been simulated. To reveal the mechanism of interaction between GHK tripeptide and Fibroblast Growth Factor, the hydrogen bonding interactions are also investigated by Molecular docking calculations. Besides, GHK-loaded Poly Lactic-co-Glycolic Acid (PLGA) nanoparticles (NPs) were synthesized with double emission (water/oil/water) method, and characterized with Zeta Sizer, UV–Vis Spectrometry, Transmission Emission Microscope and FT-IR Spectrometry. Due to the encapsulation, the shifts in the wavenumbers occurring at the characteristic peaks of GHK in histidine, peptide and carboxyl groups were also examined. The encapsulation and loading efficiencies were determined as 94% and 4%, also the in vitro release profile was performed. Peptide loaded PLGA NPs which have a spherical morphology were visualized by TEM. In vitro cell culture studies of both peptide-loaded PLGA NPs and GHK tripeptide were studied and non-toxic effect on L929 cells were found.

This study is a pioneer in the development and design of products with nano-drug formulations with better effectiveness and stability, especially in cosmetic products.