22nd Iranian Inorganic Chemistry Conference,
23-25 August, 2023
University of Kurdistan

Synthesis, characterization, computational study and covalent immobilization of H_2saldien ligand on dendrimer functionalized magnetic nanoparticles for drug delivery application

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Novel pH-sensitive, biocompatible and biodegradable magneto-dendrimers with imine and hydroxy functional groups based on polyamido-amine were synthesized for drug-delivery system that can enhance the therapeutic effects of drugs [1]. In this study, $MnFe_2O_4$ magnetic nanoparticles (MNPs) with a diameter of 35 nm were prepared by using the hydrothermal route. MNPs were coated by tetraethoxysilane (TEOS) to obtain core/shell of $MnFe_2O_4/SiO_2$. Core–shell nanoparticles were modified by (3-aminopropyl) triethoxysilane (APTES) to fabricate amine-functionalized magnetic nanoparticles (zero generation(G0)). The half generation (G0.5) of the magneto-dendrimer with methyl ester groups were produced by Michael addition reaction using the required amount of methylacrylate (MA). The first generation (G1) of nanocarrier was synthesized by the amidation reaction using the necessary amounts of N,N'-bis(salicylidene)diethylenetriamine (H_2saldien) (obtain from the reaction between salicylaldehyde (2 equiv.) and diethylenetriamine(1 equiv.)). The characterization of synthesized ligand and nanoparticles were performed by Fourier Transform Infrared spectroscopy (FT-IR), Nuclear magnetic resonance spectroscopy (NMR), X-Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-Ray Analysis (EDX), Elemental Mapping Directly from FESEM (MAP), Thermogravimetric Analysis (TGA) and Vibrating-Sample Magnetometer (VSM). Magnetic dendrimer was used as novel drug nanocarrier. Ibuprofen was chosen as model drug, which directly conjugated to imine, hydroxy and aromatic groups of terminated dendrimer by hydrogen bond and π-π stacking interaction. Drug content and drug entrapment efficiency were determined for drug-loaded nanocarrier by UV-Vis spectroscopy and in vitro drug release studies were done in simulated gastric fluid (pH=1.2), colonic media (pH=5.5), blood environment (pH=7.4) and others (pH=8.5) at 37 ºC. Such unique properties enable maintenance of the bioactivity of the drugs. Therefore, the findings in this study showed magneto-dendrimer is a promising oral drug delivery nanocarrier. This improvement could enhance the potential of magnetic targeting therapy in clinical applications of cancer treatments. Also, full optimization of the geometries of drug-loaded nanocarrier, natural bond orbital (NBO) analysis, vibrational frequencies, the HOMO–LUMO energy gap and Molecular electrostatic potential (MEP), were calculated by using density functional theory (DFT) by Gaussian software. Finally, a comparison has been made between computational and experimental results. The theoretical spectral properties show good agreement with the experimental ones.

Keywords: Magnetic nanoparticle, Magneto-dendrimer, Nanocarrier, Drug delivery, DFT study

[1] A. Esmaeili, S.N. Mousavi, *Life Sciences*, 2017, 186, 43.