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Abstract

Magnetic Nanoparticles Conjugated to Amylovis® as Contrast Agents, Synthesis and In Silico Evaluation †

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Abstract: Iron oxide nanoparticles (IONPs) have high relativity for Magnetic Resonance Imaging (MRI) and have shown a long half-life which can covalently bind with drugs and antibodies that can be used for increased contrast while imaging with MRI. IONPs are approved by the U.S Food and Drug Administration to be used as a contrast agent for MRI in vivo. The Cuban Neuroscience Center has developed a new family of naphthalene derivative compounds called Amylovis® to be used to diagnose and treatment of Alzheimer's disease (AD). The goal of this work is to synthesize IONPs with different coatings to be conjugated to Amylovis® as contrast agents for MRI. Coprecipitation method was employed to obtain the magnetic nuclei, and two synthesis methodologies were performed to coat the IONPs (post-synthesis or in situ). The different coatings used were the following: (3-aminopropyl)triethoxysilane (APTES), dicarboxylic polyethyleneglycol, galic acid, polyacrylic acid and citrate. Carbodiimide method was used as synthetic protocol to conjugate the Amylovis® moiety to different coatings. The nanoparticles were characterized by DRX, FT-IR, Electrophoretic Light Scattering (ELS) and Dynamic Light Scattering (DLS). Moreover, the stability of nanoparticles in water was evaluated using a sedimentation curve. In order to determine the potential interaction of nanosystems with the beta amyloid peptides, a molecular docking was carried out. The theoretical study showed that coatings do not affect the interaction of Amylovis® with the receptor, and the new polar groups incorporated increased the affinity to receptor.

Keywords: magnetic nanoparticles; Alzheimer's disease; MRI; IONPs; contrast agents

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