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Preparation and characterization of magnetic molecular imprinted 5-fluorouracil polymer nanoparticles based on algorithmic calculation (I)

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In targeted drug delivery, novel molecular imprinted monomers@Fe₃O₄@vinyl functional @5-fluorouracil which are prepared based on chemical affinity profiles (Hansen method) are utilized. The interaction dynamics between drug-monomer-solvent are essential in the algorithmic description for the calculation of the molecular imprinting (MIP) and the controlled drug release (CDR) components. In other words, cohesive energy density of components (CED)/resolution parameters, subparameters (δd , δp , δh) and sub-parameter combinations (δa , δv) are the basic nature of the interest profile. High chemical affinity create some difficulties in releasing controllably, however, low chemical affinity may lead to the uncontrollable and immediate releasement. According to the theoretical calculations, 4-vinylpyridine and acrylic acid were selected as desirable monomers for MIP synthesis. The synthesized MIP is utilized as a carrier for anticancer agent (5-fluorouracil) in simulated body fluid (SBF). To be detachable and transferable in body, the polymers were imprinted on the magnetic Fe₃O₄ nanoparticles (NPs) and characterized by infrared (FTIR) spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), elemental analysis (CHN) and thermal analysis (TGA/DSC/DMA). The results have shown the controllable releasement of anticancer agents.

Biography

Laleh Talavat is a PhD student in Polymer Chemistry and Graduate Research Assistant at Hacettepe University. She won awards for BAP projects, chemical affinity profiles of certain effectively used anti-cancer drugs in molecular imprinting and controlled release systems.

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