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Release of anti-cancer agent, doxorubicin, from molecular imprinted nanoparticle polymer coated multi-walled carbon nanotubes, based on chemical affinity profiles (Hansen method)(II)

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In drug-delivery systems, molecular imprinted monomers@CNT@vinyl functional is synthesized for the releasement of doxorubicin (DOX). The calculations for choosing the best reactants were done based on the utilization of chemical affinity profiles (Hansen method). The interaction dynamics between drug-monomer-solvent is the back bone in the thermodynamic calculation of the molecular imprinting (MIP) and the controlled drug release (CDR) components. Cohesive energy density of components (CED)/resolution parameters, sub-parameters (δd , δp , δh) and sub-parameter combinations (δa , δv) are the important characteristic of desired profile. High chemical affinity establish some problems in controlled release, however, low chemical affinity causes instantaneous releasement. Based on the thermodynamic computational calculations, 2-trifluoromethyl acrylic acid and (hydroxyethyl) methacrylate were chosen as optimal monomers to synthesize MIP. For controlled release of the anticancer agent, doxorubicin, in simulated body fluid (SBF) was chosen. In order to increase the release efficiency, these polymers have been imprinted on CNT nanoparticles (NPs) and were 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 illustrated the controllable release of the 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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