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## Chemical affinity profiles of certain effectively used anti-cancer drugs in controlled release systems

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In this study, multi-walled carbon nanotube (CNT) and Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles (NPs) were modified with molecular Imprinted polymer (MIP) and used as drug carriers for two anticancer agents, "Doxorubicin" and "5-Fluorouracil". Thermodynamic computation were used for both designed and released predictions and finally the controlled drug release (CDR) behaviors were investigated through. Since high chemical affinity causes difficulties in controlled release systems and low chemical affinity may lead to uncontrolled and immediate release, thermodynamic calculations is vital in drug delivery systems using MIP drug carriers. The drug-monomer-solvent interaction dynamics have a key role in the algorithmic description of the calculations for MIP and CDR components in the study. Also cohesive energy density of components (CED)/resolution parameters, sub-parameters (H-bonding, polarity and diffusion contributions) and sub-parameter combinations (H-bonding-polarity and diffusion-polarity binary contributions) and relative energy difference (RED) are the basic nature of the interest profile. In this part of study, CED profiles of monomer-drug-solvent systems have been evaluated by algorithmic approach (Hansen) to select appropriate monomers and solvent/solvent mixtures for MIP synthesis. Chemical affinity profiles have been used to design the MIP systems. In the following part of study, calculations results have been used for experimental analysis of drug release prediction.

### Biography

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

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