عنوان مقاله:

A computational method aided-molecular structure design and preparation of nano molecular imprinted polymer for extraction and quantitation of piroxicam in biological samples

محل انتشار:

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خلاصه مقاله:

In the presented work, a computational strategy was applied, in order to study the selectivity and interaction of functional monomers toward piroxicam (template) in a nano molecular imprinted polymer (MIP). In this computational approach, the binding energy of the complexes formed during the interactions between monomers and analyte of interest, was calculated. The calculated binding energies were compared, in order to design a highly selective MIP toward piroxicam. The effect of solvent on the pre-polymerization was evaluated. Electronic energies were investigated using Hartree-Fock (HF) method in MP2 level with 6-13++G(d) basis set. Based on the results obtained in this work, methacrylic acid (MAA) as functional monomer and ethylene glycol dimethacrylate (EGDMA) as crosslinking monomer were selected for synthesis of nano MIP. The designed nano MIP was applied for extraction of piroxicam prior to its determination using fluorescence spectrometry. The linearity between analytical signals and piroxicam concentration was found over the range of 31-221 µg l-3 ng mL–3 with a linear regression coefficient (R2) .of 19..6. Finally, the proposed approach was applied for trace determination of piroxicam in biological samples

کلمات کلیدی:

Computational strategy, Molecular imprinted polymer, Piroxicam, Binding energy