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Rational design and synthesis of dioxins imprinted polymer by non-covalent protocol based on computational approach

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Dioxins are a group of endocrine disrutping chemicals originate from industrial incinerators and drugs and pharmaceutical manufacturing processes. They are of concern because of their highly toxic potential at trace concentration in air and water environments, in particular, these pollutants have potential to cause reproductive and developmental problems, damage the immune system, interfere with hormones and also cause cancer. In the present work, a molecularly imprinted polymer is proposed to design for dioxins recognition at molecualr level using density functional theory (DFT) quantum mechanical simulations. The dioxin template chosen for the study was 2,3,7,8-tetrachlorodibenzo-p-dioxin or TCDD. A virtual library of 35 functional monomers was built based on interaction energy scores between the functional monomers and dioxin with B3LYP/6-31G (d) method. The interaction energy between functional monomer and the template were corrected by means of basis set superposition error (BSSE). The hydrogen bonding between dioxin and functional monomer was evaluated by changes in bond lengths before and after functional monomer-dioxin complex formation. The virtual template-monomer complex with highest interaction energy is more stable during the polymerization and it would lead in the formation of high affinity binding site for dioxin. The computational results showed that the functional monomers - methacylic acid and 4-vinyl pyridine had high energy scores while acrylonitrile was the lowest. To further compliment the computational results, the harmonic infrared and ultra-violet and visible spectroscopy were investigated. Red and blue shifts related to the stretching frequencies of either donors or acceptors of protons for hydrogen bonding were identified and compared experimentally. Stoichiometric mole ratio of template to functional monomer was optimized using Job's plots and furthermore studied the nature of the complex by UV visible spectra of the functional monomer - dioxin complex. The theoretical results were correlated by evaluation of binding parameters of MIPs. The results suggest that the proposed computational molecularly imprinting approach is a rapid, experiment-free and accurate; which would be quite useful in design of MIPs for environmental, biomedical and defense applications.

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