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Computational Design of a Dual Template Molecularly Imprinted Polymer

Multi-template imprinted polymers are attractive in application in extraction and recognition of pesticide residues in environmental matrices. Computational design was used to study intermolecular interactions in the pre-polymerization mixture between methylacryamide (functional monomer) and Carbaryl and thiodicarb (templates). The interaction energies between the computer simulated template-functional monomer complexes was calculated to provide insights on the functional monomer: Template ratio of the dual imprinted polymer. The chemical structure of the template (T) molecules {carbaryl (CBL), thiodicarb (TDC) and carbendazim (CBZ)}and the functional monomer methyl acylamide (MAM) were drawn using Gauss view 5.0 and saved as Gaussian input files. The template and functional monomer were then subjected to geometry optimization at DFT level using B3LYP/6-31G(d) then subjected to optimization and frequency calculations at the same level. The frequencies were examined to ensure that the conformations correspond to a minimum on the potential energy curve. The electronic energy of the system was used for energy calculation of the complex formed. The value of change in energy (ΔE) was subsequently analyzed and used to predicts the most stable complex. The complexes exhibited negative interaction energy (ΔE) whose magnitude increased as the monomer: template ratio increases for both CBL and TDC and could be used to evaluate the imprinting process. It is observed that when higher amounts of functional monomer are used, the effect of steric crowding was exhibited by the TDC: MAM ratio 1:4 which resulted in high positive energy change that imply instability, on the other hand CBL-MAM still exhibited a large negative energy change implying greater stability. The results indicate the optimal molar ratio for the synthesis of the dual template MIP using MAM is 1: 3. The complexes of the two templates exhibited equal interaction energy at this ratio. Therefore, a computational approach can be used in designing multi-template imprinted polymers.

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