Molecularly Imprinted Polymer and Computational Study of (E)-2-Cyano-3-(Dimethylamino)-N-(2,4-Dioxo-1,2,3,4-Tetrahydropyrimidin-5-Yl)Acrylam-Ide and Its Applications in Industrial Applications

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Abstract : In this investigation, the (E)-2-cyano-3-(dimethylamino)-N-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)acrylam-ide (4) which used TAM as a template which interacts with Methacrylic Acid (MAA) monomer, in the presence of CH_3CN as progen. The TAM-MMA complex interactions are dependent on stable hydrogen bonding interaction between the carboxylic acid group of TAM(Template) and the hydroxyl group of MMA(methyl methacrylate) with minimal interference of porogen CH_3CN. The physical computational studies were used to optimize their structures and frequency calculations. The binding energies between TAM with different monomers showed the most stable molar ratio of 1:4, which was confirmed through experimental analysis. The optimized polymers were investigated in industrial applications.

Keywords : molecular imprinted polymer, computational studies, SEM, spectral analysis, industrial applications

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