Theoretical Screening and Selection of Functional Monomers for Molecular Imprinted Electropolymer as Sensor for Glutamate

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Neurotransmitter glutamate excess release caused overstimulation of brain called excitotoxicity resulting in cell death, ischemic stroke and certain neurodegenerative diseases viz., epilepsy, amyotrophic lateral sclerosis, Alzheimer's, and Parkinson's disease. Using molecular imprinted polymer as synthetic receptor, we can develop functional MIP with predetermined selectivity for various templates especially for neurotransmitters. It relies largely on the molecular recognition through the functional monomer and template interactions. So, a theoretical model for suitable selection of functional monomer for synthesizing molecular imprinting electropolymers (MIPs), with specific recognition for detection of glutamate, a key neurotransmitter involved in neuronal diseases is attempted. Here, the density functional (DFT) method with the hybrid B3LYP exchange-correlation functional has been applied to investigate the intermolecular interactions between glutamate and several functional monomers viz., pyrrole, 3,4-ethylenedioxythiophene (EDOT), o-phenylenediamine (o-PD), thiophene, aniline and 3-aminophenyl boronic acid (3-APBA) most commonly used in the preparation of conducting MIPs. The most stable configurations of the glutamate, functional monomers and complexes formed were considered for analysis. The geometrical, vibrational and NMR chemical shift parameters involving hydrogen bonding sites of the most stable interacting systems have been analysed. Our results illustrate that, among the different glutamate/monomer molecular systems considered, the binding energies between glutamate and functional monomers are in the order, 3-APBA > pyrrole > aniline > o-PD > thiophene > EDOT. The stronger binding interactions of 3-APBA suggests it as an efficient monomer for selective functional MIP based sensors for glutamate.

Keywords: BINDING ENERGY; DENSITY FUNCTIONAL THEORY; H-BONDING INTERACTION; MOLECULAR IMPRINTED ELECTROPOLYMER; NEUROTRANSMITTER