FIRST-PRINCIPLES INSIGHTS INTO THE DESIGN OF MOLECULARLY IMPRINTED POLYPYRROLE FOR DETECTION OF CLORSULON

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Molecularly imprinted polymers (MIPs) are artificial receptors designed to selectively recognise a specific target molecule. They are created by polymerising functional monomers in the presence of the analyte, resulting in a polymer matrix containing cavities complementary to the target, also called template [1]. The synthesis of MIPs includes the selection of suitable functional monomer and solvent, polymerisation, removal of the template, and evaluation of MIP sensitivity and selectivity through rebinding. These steps are time-consuming and costly, and the complexity of experiments requires deeper insights to overcome the challenges [2]. Semi-empirical metadynamics and density functional theory (DFT) were employed to calculate the molecular modelling properties. The electronic and physicochemical properties of polypyrrole conformers under αβ- and ββ-coupling of monomers were studied. The optimal imprinting conditions, including the best solvent and optimised monomers to template ratio, were calculated. The sensing mechanism of clorsulon through binding sites was described with density of states (DOS), UV-vis spectroscopy, and charge transfer analyses of optimised molecular systems. The study showed the binding sites had different sizes and densities, indicating variation of binding affinities and surface areas. At the optimised condition calculated, imprinted polypyrrole shows properties that promise a real-time sensing empowered with improved selectivity and sensitivity towards clorsulon.

[1] E. Mohsenzadeh et al., “Application of computational methods in the design of molecularly imprinted polymers (review),” TrAC Trends in Analytical Chemistry, vol. 171, p. 117480, Feb. 2024, doi: 10.1016/j.trac.2023.117480.

[2] G. Zvirzdine et al., “Electrochemical Salicylic Acid Sensor Based on Molecularly Imprinted Polypyrrole,” ACS Appl. Mater. Interfaces, vol. 17, no. 41, pp. 57475–57485, Oct. 2025, doi: 10.1021/acsami.5c11951.