Bio-inspired functionalization of chitosan for water remediation: computational insights into neonicotinoid sequestration

Jorge M. C. Marques[1], Joana R. C. Santos[1], Paulo E. Abreu[1]

[1]*CQC-IMS, Department of Chemistry, University of Coimbra, Portugal*
qtmarque@ci.uc.pt

Computational techniques can significantly enhance the design of materials with high adsorption affinity for target molecules, a capability crucial for the sequestration of pesticides in water remediation. This work employs a multi-stage computational protocol[a] to guide the design of bio-inspired, chitosan-based materials for the efficient adsorption of neonicotinoids, including imidacloprid, thiacloprid, acetamiprid, clothianidin, and dinotefuran (considering both *R*- and *S*-enantiomers). By employing molecular dynamics (MD) simulations, we investigated the interactions between these pesticides and the *Aplysia californica* acetylcholine-binding protein (*Ac*-AChBP) to identify key amino acids responsible for stabilizing the protein-pesticide complexes within the binding pocket. High-level electronic-structure calculations were subsequently performed on isolated residues, identifying tryptophan (Trp) and tyrosine (Tyr) as the most promising candidates for functionalizing chitosan. The adsorption efficiency of these functionalized models was evaluated against non-functionalized chitosan through comparative MD simulations in aqueous media. Our results demonstrate that the incorporation of aromatic amino acids significantly enhances the adsorption properties of chitosan, especially for imidacloprid, acetamiprid, and thiacloprid. This integrated computational strategy provides a robust framework for selecting molecular targets to improve the performance of biodegradable natural resources in environmental applications.

References:

[a]Santos, J. R. C.; Abreu, P. E.; Marques, J. M. C. Towards nature-inspired materials for adsorbing pesticides: a multi-stage computational approach. Phys. Chem. Chem. Phys., 2025, 27, 18665-18680. https://doi.org/10.1039/D5CP01445J