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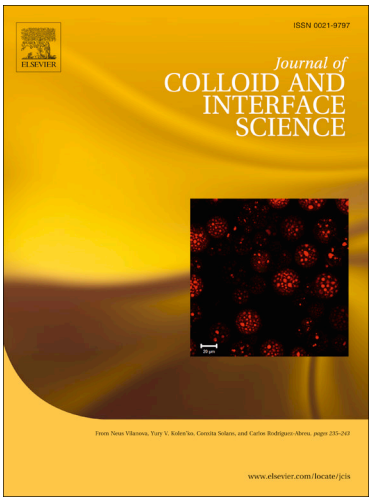

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POLYDIACETYLENE FUNCTIONALIZED WITH CHARGED TERMINI FOR DEVICE-FREE COLORIMETRIC DETECTION OF MALATHION

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Abstract

We introduce 10,12-Pentacosadiynoic acid conjugated with pyridine-2-aldoxime (pralidoxime, PAM) as a positively charged amphiphilic molecule capable of forming a polymer with polydiacetylene (PDA-PAM) via 1,4-addition photopolymerization of self-assembled PAM-modified monomers. Colloidally stabilized vesicles formed by PDA-PAM and unmodified pentacosadiynoic acid via electrostatic interactions in a basic aqueous medium exhibit a colorimetric transition in the presence of malathion. The malathion detection limit, through color change observed by the naked eye, is in the mM range (liquid suspension) or at nmol/cm^2 levels (solid membrane); the response to exposure to malathion was rapid, within seconds. Density functional theory (DFT) calculations on the PDA-PAM system before and after binding with the target molecule (malathion) demonstrate that the large blue absorption shift of 0.42 eV observed in the malathion-bound configuration of the polymer is due to the dissociation of the positive charge center on the pralidoxime functional group from the negative charge center on the carboxylic terminus.