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Investigating the structure-activity relationship of amphiphilic nucleophiles to hydrolyze major classes of pesticides in micellar medium

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Pesticides/insecticides have been used by mankind since times immemorial to control pests and mosquitoes. They are also used by industries as solvents, plasticizers, flame retardants and are present as major ingredient of commercially available insecticides. This means that every person gets exposed to these chemicals in some form, during his/her life time. Due to their high penetration via oral, inhalation and/or dermal route and long biological half-life, these toxic chemicals can cause severe health effects over chronic exposure. Their toxicity is well noticed as chemical warfare agents and their mechanism of toxicity is due to the irreversible binding to serine residue of enzyme Acetylcholine Esterase (AChE) lending it incapable of Acetylcholine (Ach) recycling at neuronal synapse Herein, we are using oxime-based chemistry to synthesize para and ortho amphi oxime catalysts that show high hydrolytic activity against the different classes of pesticides in micellar medium. The rate constant values of amphiphilic catalysts show that the positioning of oxime group in the structure contributes to their activity in the micellar condition. Amongst all the catalysts, ortho-amphi oxime proves to be the most potent catalyst which shows 10-fold higher activities than para-am phi oxime. The conjugation of aliphatic chain to ortho and para-oximes enhance their interaction with the cationic surfactant helping in decreasing their pKa value and make it more reactive around physiological pH. In future, these amphiphiles can be commercially formulated into spray/cleansing solution to decontaminate insecticides/pesticides present on the surfaces.

Biography

Subhashini Pandey is a PhD student in the Laboratory of Self-Assembled Biomaterials, INSTEM-NCBS, Bangalore, India. She has completed M.Tech, in Chemical Engineering at Dr. B.R. Ambedkar National Institute of Technology (Jalandhar), and thesis work in Dr. Vemula's lab. After completing her thesis work, she has received prestigious Lady Tata Merorial Trust fellowship for pursuing for PhD work in Praveen's lab.

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