Enhancing Pesticide Detection: The Role of Serine in Lipopeptide Nanostructures and Their Self-Assembly Dynamics

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In this research, we introduced serine into a novel lipopeptide sequence to optimize the detection capabilities for organophosphate pesticides, specifically glyphosate [1,2]. The revised sequence features a hydrophilic region composed of proline, arginine, tryptophan, and glycine (PRWG) alongside a hydrophobic segment with one or two alkyl chains (Table 1). The study comprehensively explored how serine incorporation influences the physicochemical properties and supramolecular assembly of the lipopeptides, leading to enhanced interactions with glyphosate. Advanced analytical methods were employed to investigate these modifications, including fluorescence spectroscopy, circular dichroism, and small-angle X-ray scattering (SAXS). The results showed that serine significantly reduces the critical aggregation concentration, increases the hydrophilicity of the lipopeptides, and promotes the formation of distinct secondary structures—alpha-helices in molecule **1** and beta-sheets in molecule **2**. Moreover, isothermal titration calorimetry (ITC) and density functional theory (DFT) calculations confirmed the improved binding affinity with glyphosate. Molecule **1**, with one alkyl chain, demonstrated notably higher catalytic activity and sensitivity, marking it as particularly effective for acetylcholinesterase mimicry in pesticide detection (Table 1). This enhancement suggests that serine-functionalized lipopeptides have great potential as biomimetic sensors in environmental monitoring.

Table 1. Lipopeptides used in this work and their corresponding theoretical and experimental molecular weights (M_w).

	Chemical Composition	Experimental M_w (g mol^{-1})	Linear region (µmol L^{-1})	LOD (µmol L^{-1})	Sensitivity	Reference
1	SPRWG-$(CH_2)_{17}CH_3$	853.17	1-3	0.3	1.29	This work
2	SPRWG-$[(CH_2)_{17}CH_3]_2$	1105.64	1-1200	64	0.15	This work
3	PRWG-$(CH_2)_{17}CH_3$	766.65	1-12	0.3	0.12	[1]
4	PRWG-$[(CH_2)_{17}CH_3]_2$	1018.86	1-60	1.5	0.09	[1]

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References

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