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# In silico design and experimental validation of peptidic Self-Assembled Monolayers

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Self-Assembled Monolayers (SAMs) are constituted by small molecules that chemisorb on specific surfaces and spontaneously assemble as an ordered layer. In particular, the recently developed peptide-based SAMs can be exploited in biological applications thanks to their intrinsic biocompatibility. In this study we use atomistic simulations to characterize peptidic SAMs on gold surface to design the best amino acid sequence for biological application. The investigated peptides feature a headgroup (Cysteine, for thiolate bond formation with gold), a linker formed by a sequence of 1 to 4 amino acids (chosen between A, F, G, P, S, Y), a zwitterionic layer formed by an alternation of opposite charged residues (KEn), and an integrin binding end group (GRGDSP). In the first screening we test the formation of secondary structures in isolated peptides using Replica Exchange simulations and validating the results by Circular Dichroism. The most promising peptides are then simulated in SAM configuration on gold surface and analyzed in terms of secondary structure, tilt angle, lateral interactions formation, hydrophilicity, height and RGD exposure to solvent. The results show that the optimal peptide needs a linker of 3 residues of Proline or Phenilanaline and a layer of at least 4 KE pairs.