Title:	Ordering Transitions in Liquid Crystals Triggered by Bioactive Cyclic Amphiphiles: Potential Application in Label-Free Detection of Amyloidogenic Peptides
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Abstract:	We report the orientational behavior of nematic liquid crystals (LCs) influenced by a cyclic lipopeptide, polymyxin B (PmB). It was found that PmB can spontaneously self-assemble at aqueous-LC interfaces and induce a homeotropic ordering of the LCs at those interfaces, thus resulting in dark optical appearance of the LC under cross polarizers. Density functional theory studies substantiate the experimental findings that the stability of homeotropic anchoring of the LC is strongly influenced by the hydrophobic interactions between aliphatic tails of PmB and LC molecules along with the additional supramolecular interactions between their head groups. Interestingly, exposure of the PmB-laden aqueous-LC interface to anionic serum proteins such as bovine serum albumin (BSA) and human hemoglobin triggered a planar reorientation of the LC, leading to a bright optical state of the LC. This allows label-free characterization of the biomolecular interactions between proteins and antibiotics (i.e., PmB) in vitro at those interfaces. Such peptidic (PmB)-based LC interfaces can also distinctly amplify the adsorption of β-sheet-rich proteins (fibronectin and concanavalin A) through appearances of fibril-like spatial patterns which are, however, not observed in the presence of α-helix-rich proteins (BSA). Such changes in the optical patterns of the LC in contact with β-sheet-rich proteins occur at nanomolar concentrations at those interfaces, and thus the method could be useful to detect toxic amyloids at a low concentration regime. We envision that our simple label-free optical system may open a wide avenue to detect an extensive assortment of interfacial biochemical events occurring at the aqueous-LC interfaces.
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