

Probing chiral interactions between L- and D-arginine-based polymers and sodium deoxycholate solutions

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Nowadays the spontaneous self-organization of a polymer into an ordered structure is a sought-after property of many smart materials, whose applications might range from catalysis [1] to drug-delivery [2]. However, literature regarding the role played by these specific conformations in chiral recognition remains scarce. In this context, polyamidoamino acids (PAACs) are an emerging class of stimuli-responsive bioinspired synthetic polymers able to self-assemble into pH depend conformations [3,4]. PAACs are an off-spring of polyamidoamines (PAAs), a family of polymers obtained by the Michael-type polyaddition of *prim*-monoamines or *sec*-diamines with bisacrylamides. The reaction occurs in aqueous solution at pH = 8–9 and at room temperature. By using α -amino acids as monomers, PAACs are obtained.

The first example of PAAC was named ARG07, obtained by the stepwise polyaddition in water of L- or D-arginine to *N,N'*-methylenebisacrylamide. Results indicated M_n 8500, PDI 1.4 and R_h of 1.2 nm [3]. Molecular dynamics (MD) and circular dichroism (CD) showed ARG07 folded into a rigid structure, reminiscent of the hairpin conformation, solely driven by the polymer main chain. Due to its ability to self-assemble in solution forming chiral structures, L- and D-ARG07 may selectively interact with biological components.

To assess chiral recognition, sodium deoxycholate (NaDC), one of the components of bile salts, was chosen as a chiral model surface. In aqueous solution, NaDC showed three different pH dependent behaviour: homogeneous solution (pH>8), gel phase (pH 7-8) and aggregation/flocculation (pH<6.5). Notwithstanding the ability of NaDC to self-assemble into different conformations at each pH interval, signs of chiral recognition were found in NaDC gel phase only. Conformational modifications were probed by circular dichroism spectroscopy: both D- and L-ARG07 changed shape and magnitude of the CD pattern, whereas D,L-ARG07 did not modify the CD spectra of NaDC. After 8 days, NaDC compact structure loosened, ended up being fluid and the CD pattern were completely modified due to NaDC and D- or L-ARG07 interactions. Incoming diffusion NMR and SANS studies will probably highlight the mechanisms and dynamics of the chiral interactions in these polyelectrolyte-micelle systems.

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Biography(100 Words)

Federica Lazzari is currently enrolled in the Industrial Chemistry PhD program of the University of Milan, Italy. During the last three year she worked on the synthesis and determination of the self-assembly ability, chiro-optical and solution properties of a new class of α amino-acid deriving polymers. During her PhD, she worked with Prof. Peter Griffiths from University of Greenwich, UK. The project was focused on probing conformational modifications and enantiomeric selections in bile salts micelles,

through circular dichroism and pulsed gradient spin echo NMR. Prior to her PhD, she obtained her MSc in Industrial Chemistry, in the University of Milan.

