Dissecting Self-folding Process of Curved Supramolecular Polymers

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Intrachain folding of proteins enables their main chains to form specific high-order structures, which are essential for biological functions.[1] For supramolecular polymers (SPs), one-dimensional molecular assemblies formed through non-covalent bonds, replicating the folding remains challenging due to difficulty in embedding additional interaction sites that can guide folding the main chains.[2] Our group reported that barbituric acid-incorporated derivative **1** can form hydrogen-bonded macrocycles (rosettes), and the resultant rosettes stack via π–π interaction to afford SPs with helically folded (helicoidal) and randomly coiled domains in a main chain. Interestingly, upon aging the SPs solution, highly folded helicoids can be obtained through self-folding process of randomly coiled domains by using helicoidal domains as template to result in highly folded helicoidal SPs.[3]

Based on the above study, we herein newly synthesized and explored self-assembly of compound **2** possessing two naphthalene rings (Figure 1a). Under thermodynamic condition achieved by temperature-controlled protocol, **2** formed highly folded helicoidal SPs through self-folding similarly to **1** (Figure 1b, left). On the other hand, kinetic condition by rapid solvent mixing protocol afforded linearly extended fibers (Figure 1b, right). Time-dependent AFM observations and spectroscopic measurements demonstrated that the linear fibers could partially self-fold to form curved domains but via a complex process. We discuss these two distinct self-folding processes of the SPs obtained from **2**.

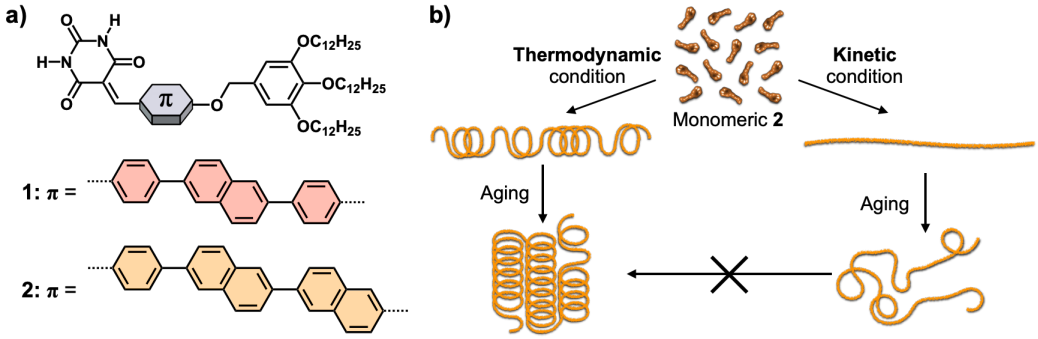

Figure 1. a) Chemical structure of compound **1** and **2**. b) Schematic representation of folding processes of SPs obtained from **2**.

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