Supporting Information

Antibody-Mimetic Peptoid Nanosheets for Molecular Recognition

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Contents

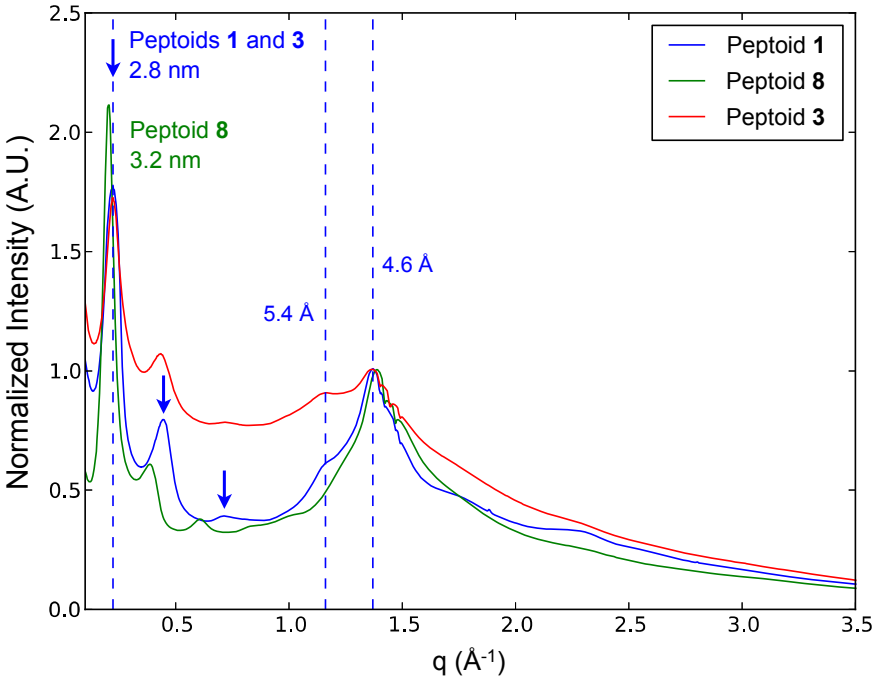

Figure S1. Powder X-ray diffraction spectrum of a dry, pelleted stack of nanosheets prepared from either: **1** (blue), **8** (green), or **3** (red). The spectra are normalized by the intensity of the 4.6 Å peak, thereby revealing the noticeably higher intensity exhibited by **3** in the q = 0.25 $Å^{-1}$ to 1.5 $Å^{-1}$ range which is attributed to diffuse scattering from the randomly oriented, disordered loop domains of **3**. The three equally spaced peaks (denoted by blue arrows) arise from the 2.8 nm thickness of the Peptoid **1** bilayer.

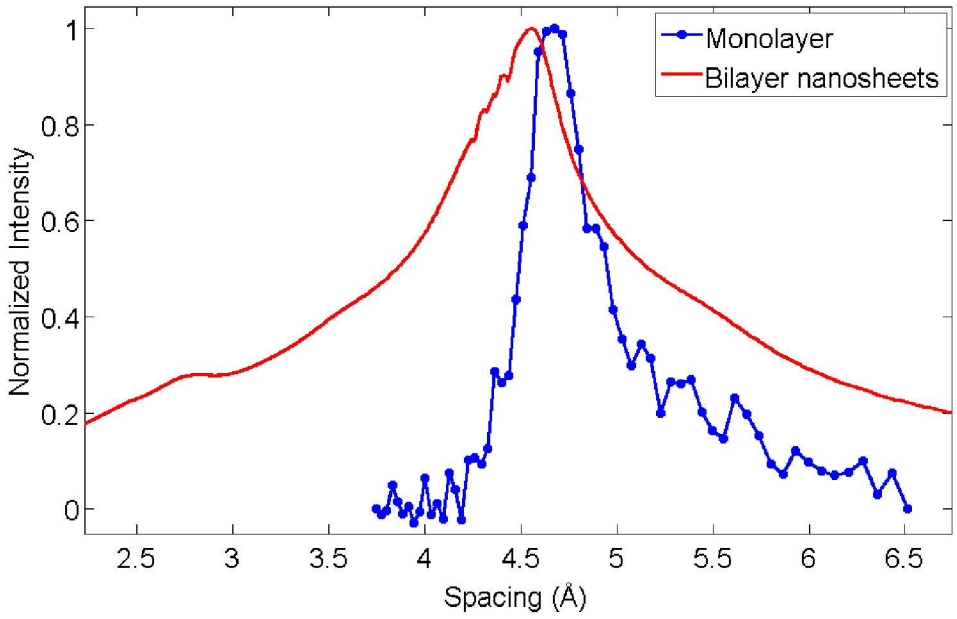

Figure S2. Comparison of the grazing incidence X-ray diffraction peak obtained from the Peptoid **3** monolayer at the air-water interface, after compressing the monolayer to a fixed surface pressure of 37 mN/m (blue), and the powder X-ray diffraction peak obtain from a dry pellet of Peptoid **3** nanosheets (red), at the 4.6 Å spacing, corresponding to the lateral distance between neighboring polymer chains.

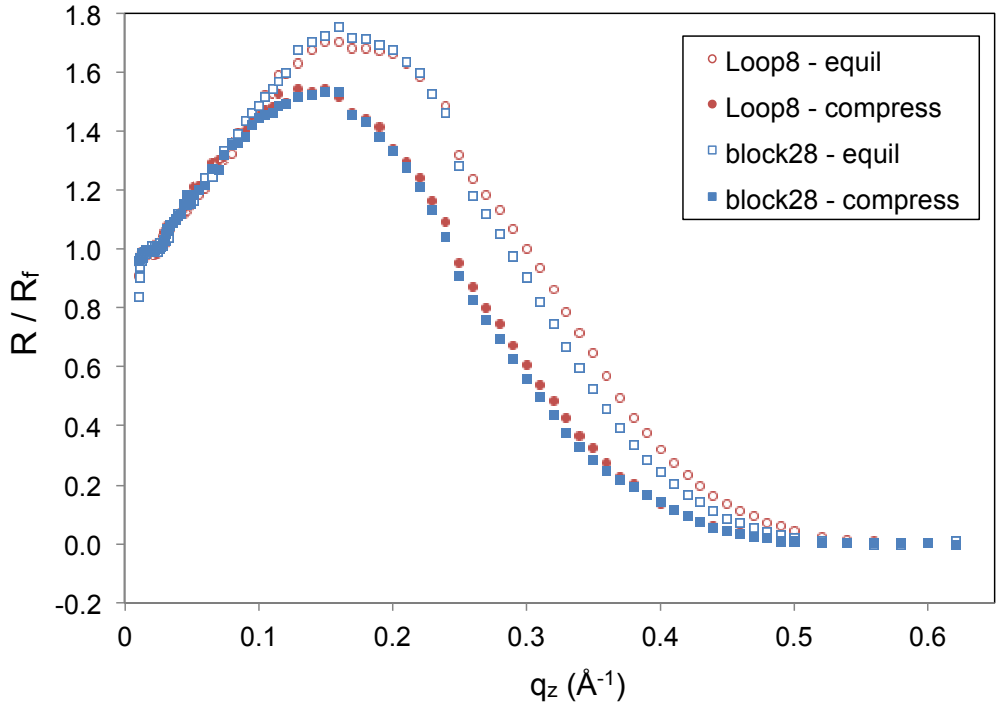

Figure S3. Fresnel-normalized reflectivity data obtained from the Peptoid **1** (blue) and **3** (red) monolayers at equilibrium surface pressure (open symbols) and after compressing each peptoid monolayer to a fixed surface pressure of 37 mN/m (closed symbols). Error bar (vertical line), corresponding to the standard deviation, is included with each point.

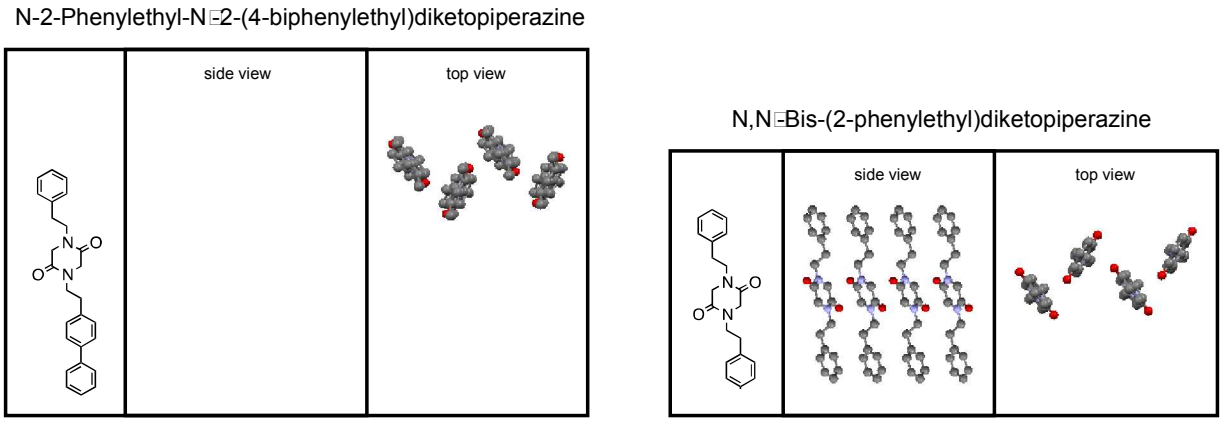

Figure S4. Diketopiperazine (DKP) crystal structures, for predicting aromatic packing of phenylethyl and biphenylethyl sidechains within the nanosheets. The crystal structure of compound **9** (shown at left) is compared with that of N,N'-Bis-(2-phenylethyl)diketopiperazine (right), previously reported by Murnen et al.[1] Compound **9** was synthesized as previously described[1] and then crystallized from chloroform. Crystal structures were determined at UC Berkeley's CheXray facility. The crystal structure file (4-Biphenylethyl-2-phenylethyl-DKP.cif) for compound **9** is available in Supporting Information.

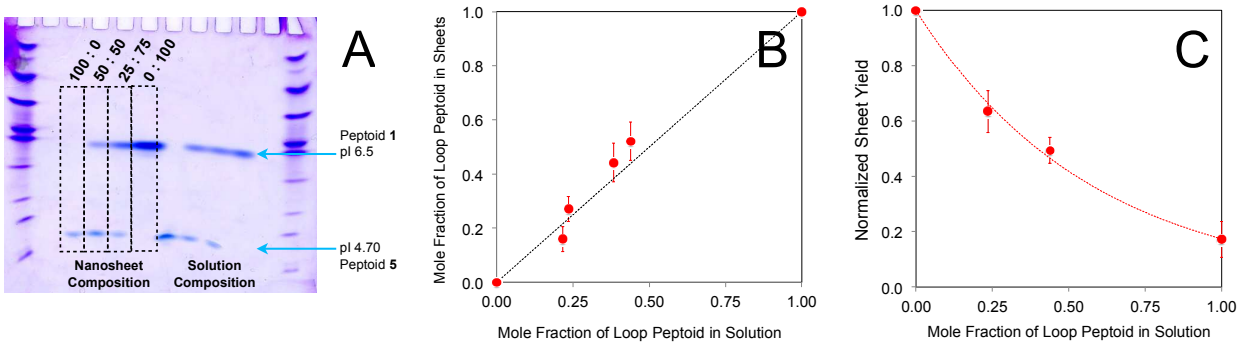

Figure S5. Quantification of the fractional composition of two-component peptoid nanosheets by denaturing the nanosheets into free polymer strands with 0.2% sodium dodecyl sulfate and measuring the relative amount of each strand present in the mixture using isoelectric focusing (IEF) gel electrophoresis. (A) Representative IEF gel image, used for quantification. Lanes 1 and 12 of the gel contain the IEF protein standard. The intensity of the Peptoid **1** and **5** bands in the gel was quantified with ImageJ software and used to calculate the fractional percentage (mole fraction) of each compound present in a given nanosheet preparation. Nanosheet yield was computed as the sum of the intensities of the band(s) appearing in a given lane of the gel. (B) Correlation between solution composition and nanosheet composition for nanosheets made from peptoid solutions containing different mixing ratios of **1** and **5**. (C) Impact of the two-component mixing ratio on nanosheet yield, normalized by the yield obtained with 0 mol-% Peptoid **5** (pure **1**) nanosheets. In panels B and C, the axis label of Loop Peptoid is synonymous with Peptoid **5**.

References

[1.] Murnen, H.K.; Rosales, A.; Jaworski, J.N.; Segalman, R.A.; Zuckermann, R. N. Hierarchical Self-Assembly of a Biomimetic Diblock Copolypeptoid into Homochiral Superhelices. *J. Am. Chem. Soc.* **2010**, *132*, 16112–16119.