Electronic Supplementary Material (ESI) for Nanoscale.

Self-assembly Dynamics and Antimicrobial Activity of All L- and D-amino Acid Enantiomers of a Designer Peptide

Zhou Ye[a], Xiao Zhu[a,b], Sergio Acosta[c], Dhiraj Kumar[a], Ting Sang[a,d], Conrado Aparicio[a]*

a MDRCBB, Minnesota Dental Research Center for Biomaterials and Biomechanics, University of Minnesota, Minneapolis, Minnesota 55455, United States

b The State Key Laboratory Breeding Base of Basic Science of Stomatology & Key Laboratory of Oral Biomedicine Ministry of Education, School of Stomatology, Wuhan University, Wuhan 430079, China

c G.I.R. Bioforge, University of Valladolid, CIBER-BBN, Paseo de Belén 11, 47011 Valladolid, Spain

d Jiangxi Provincial Key Laboratory of Oral Biomedicine, School of Stomatology, Nanchang University, Nanchang 330006, China

*apari003@umn.edu

Critical aggregation concentration by Nile Red assay

Nile Red has high affinity to the hydrophobic region of the self-assembled peptide nanofibers. In aqueous solution without hydrophobic environment, the fluorescent signal is very weak[1]. Nile Red concentrated stock solution was prepared at 2 mM in methanol and was then diluted in pH 10.8 borax-NaOH buffer to a final concentration of 1 μM. L-GL13K stock solution was prepared at 20 mM in DI water and was diluted in pH 10.8 borax-NaOH buffer to the concentration range of 0.2 μM-1 mM. Equal volume (100 μl) of 1 μM Nile Red solution and L-GL13K solution at different concentration was added and mixed in 96-well black microplates. The fluorescence assay was conducted at an excitation wavelength of 530 nm and an emission wavelength of 590 nm using a BioTek Synergy HT microplate reader (Winooski, VT, USA). The fluorescence intensity was plotted against the logarithm of L-GL13K concentration. When the concentration was close to the critical aggregation concentration, a sharp increase in the intensity should be observed due to the hydrophobic environment.

Reference:

1 R. M. P. Da Silva, D. Van Der Zwaag, L. Albertazzi, S. S. Lee, E. W. Meijer and S. I. Stupp, *Nat. Commun.*, , DOI:10.1038/ncomms11561.

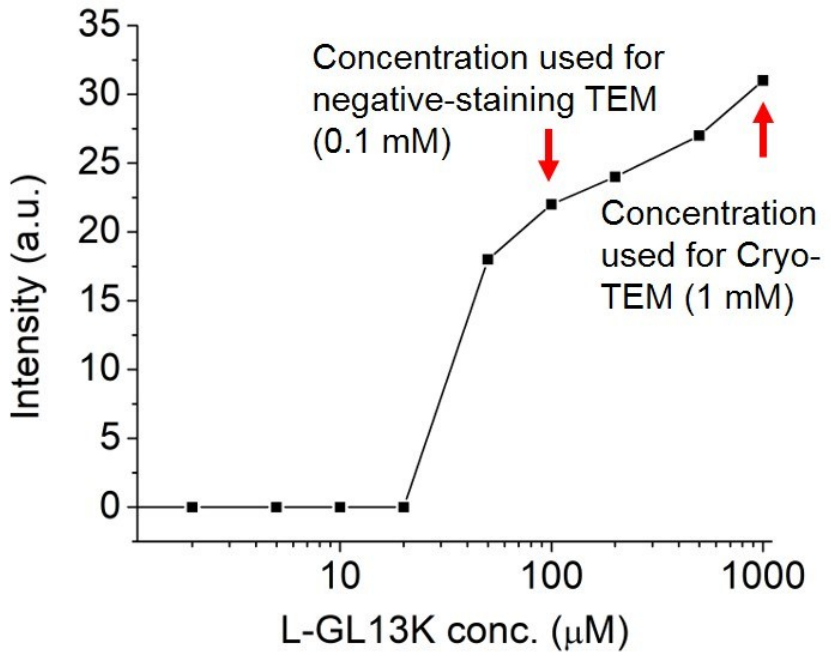

Figure S1. Nile Red assay of L-GL13K at the concentration range of 0.2 μM to 1.0 mM. The critical aggregation concentration was between 20 to 50 μM.

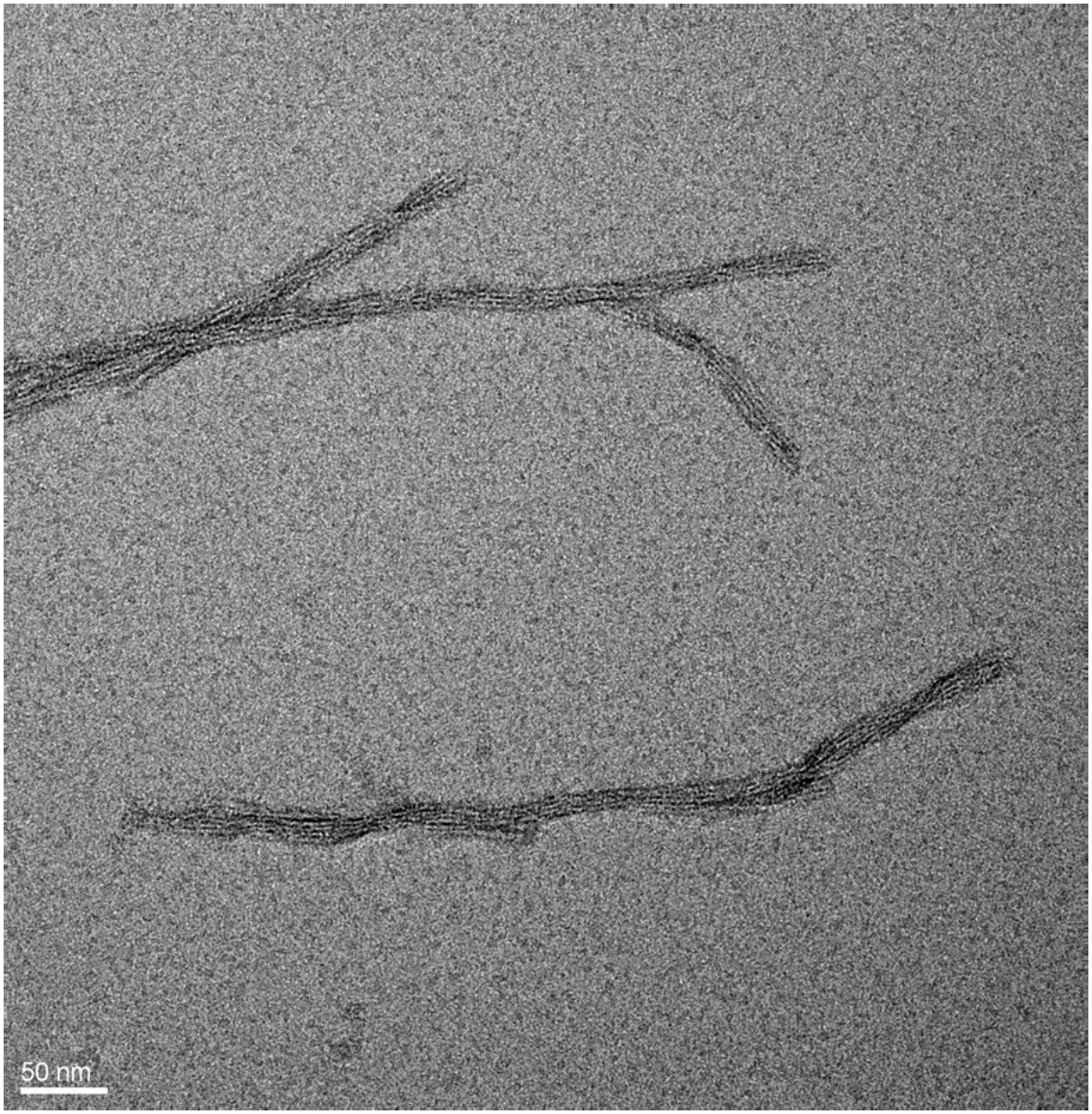

Figure S2. High-resolution TEM image of 0.1 mM L-GL13K in pH 9.8 borax-NaOH solution for 8 days.

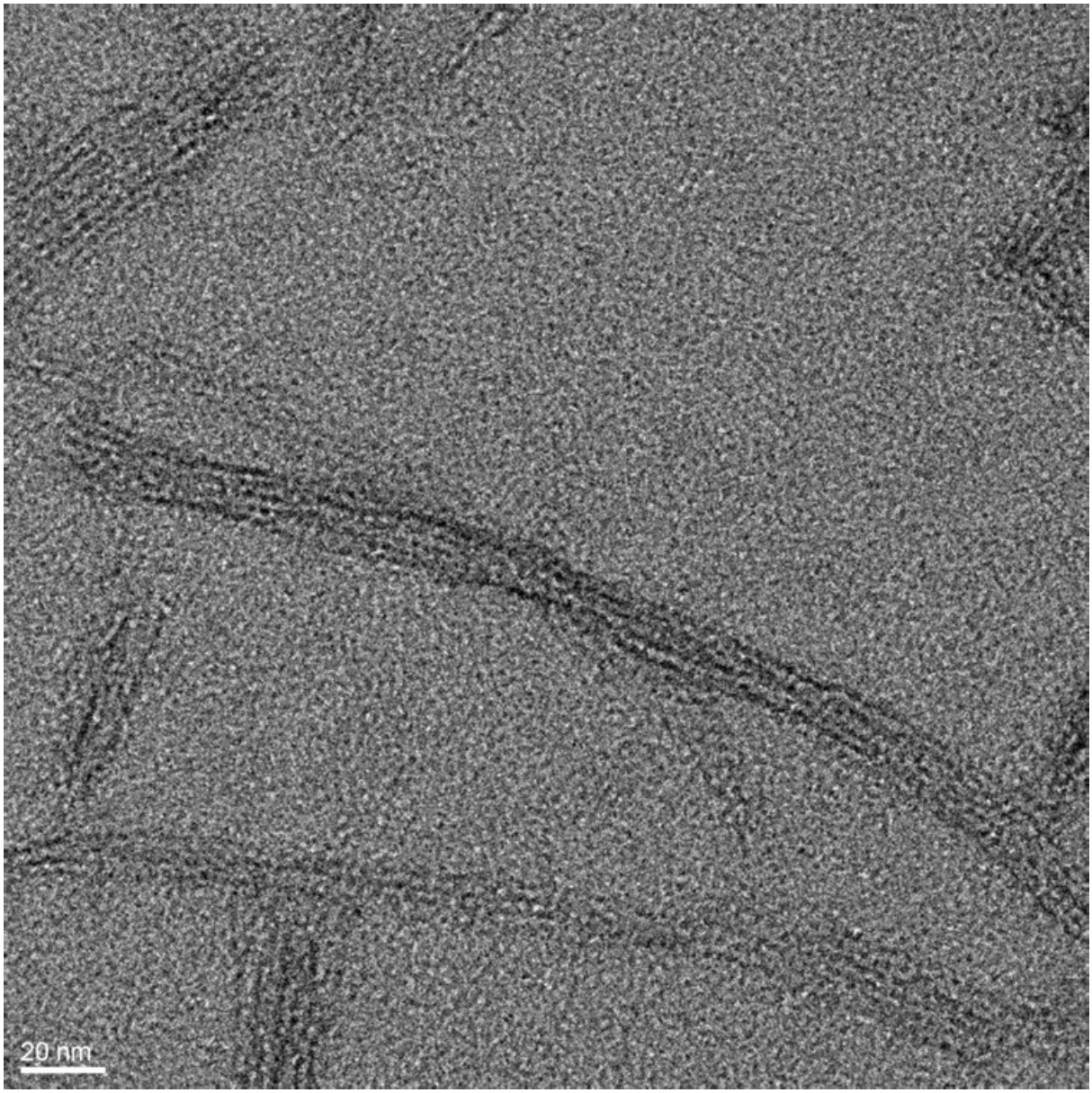

Figure S3. High-resolution TEM image of 0.1 mM L-GL13K in pH 10.8 borax-NaOH solution for 2 days.

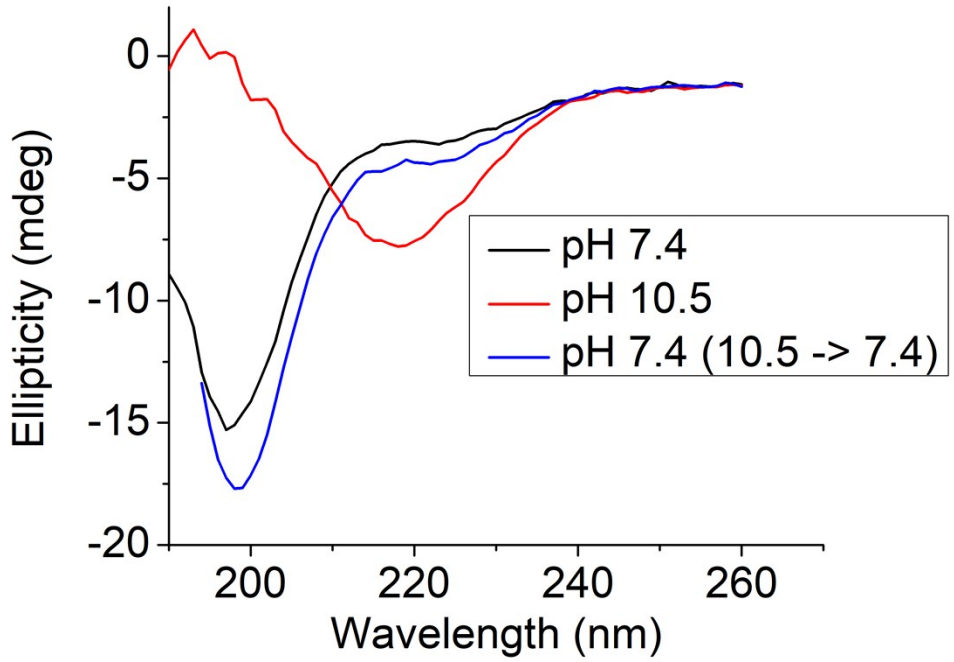

Figure S4. CD spectra of 0.1 mM L-GL13K in buffer solutions at pH 7.4, pH 10.5 and titrated from pH 10.5 to pH 7.4.

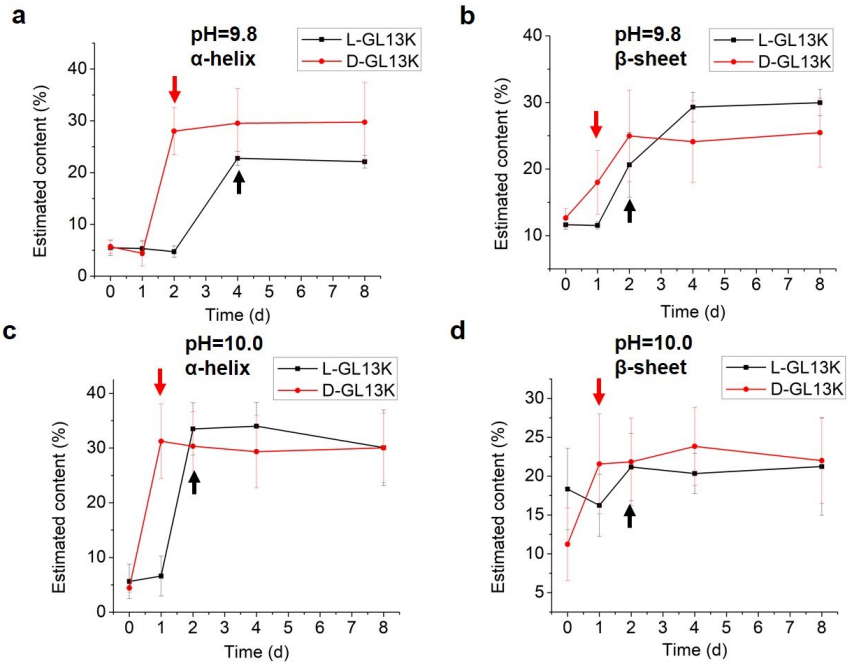

Figure S5. Estimation of secondary structure (a, c, α-helix; b, d, β-sheet) contents of L- and D-GL13K in pH 9.8 and pH 10.0 solutions for up to 8 days. The time for sharp increase in content change was marked by black (L-GL13K) and red (D-GL13K) arrows.