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## Molecular Packing and the Handedness of the Self-assemblies

## of C17H35CO-Ala-Phe Sodium Salts

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**Fig. S1** Pictures of the hydrogels at a concentration of 30 g L<sup>-1</sup> at room temperature.

**Table S1** Minimum gelation concentrations (MGCs) of the lipodipeptide sodium salts in deionized water.<sup>a</sup>

Lipodipeptide	<b>MGC (</b> g L⁻¹)
(L, L)- <b>8</b>	23.5
(L, D)- <b>8</b>	21.5
(D, L)- <b>8</b>	21.0
(D, D)- <b>8</b>	24.0

<sup>a</sup>The formation of stable hydrogels was determined by the tube inversion method. Each lipodipeptide sodium salt and 1 mL of  $H_2O$  was heated to obtain a clear and transparent aqueous solution in a test tube. Then, the tube was put into a 25 °C-thermostatic waterbath for 1 h.

Table S2. MGCs of the	lipodipeptide sodium	salts in selected organic solvents.	b
		0	

	MeOH	EtOH	<i>n</i> -PrOH	toluene	THF	DMF	DMSO
(L, L)- <b>8</b>	-	-	-	15	16	14	12
(L, D)- <b>8</b>	-	-	-	15	17	15	14
(d, l)- <b>8</b>	-	-	-	17	18	14	12
(D, D)- <b>8</b>	-	-	-	16	16	13	11

<sup>*b*</sup>The data in the above table refer to the MGCs (g L<sup>-1</sup>) of the lipodipeptide sodium salts in the listed organic solvents at 25 °C. -: Solution, no gelation occurred at a concentration of 30 g L<sup>-1</sup>.



Fig. S2 CD spectra of the hydrogels at a concentration of 30 g  $L^{-1}$  at 25 °C.



**Fig. S3** FT-IR spectra of the aqueous solutions and hydrogels of (L, D)-8 and (D, D)-8 in  $D_2O$  at a concentration of 30 g L<sup>-1</sup>.



**Fig. S4** <sup>1</sup>H NMR spectra of (D, D)-**8** and (L, D)-**8** hydrogels (25 g L<sup>-1</sup>) and solutions (5 g L<sup>-1</sup>) in  $H_2O/D_2O$  (v/v = 90/10).



Fig. S5 SAXRD patterns of the xerogels of (a) (L, D)-8 and (b) (D, D)-8.



Fig. S6 WAXRD patterns of the xerogels of (a) (L, D)-8 and (b) (D, D)-8.