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Supporting information for article:

Spatiotemporal control of l-phenylalanine crystallization in microemulsion: the role of water in mediating molecular self-assembly

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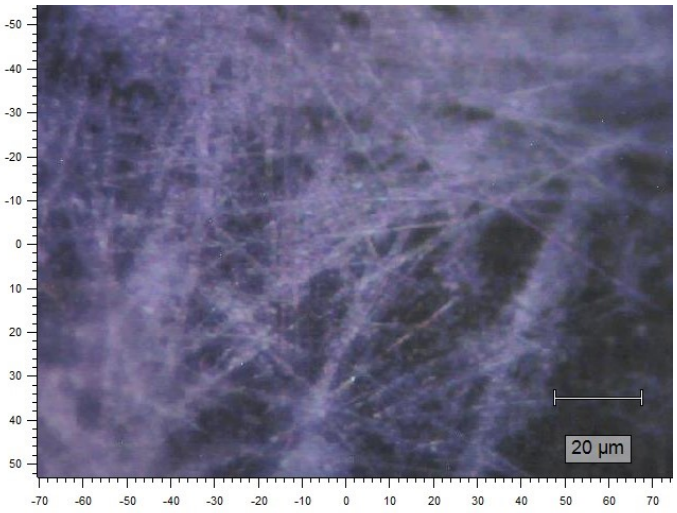

Figure S1 The images of crystalline fibril structure measured by laser confocal Raman spectroscopy.

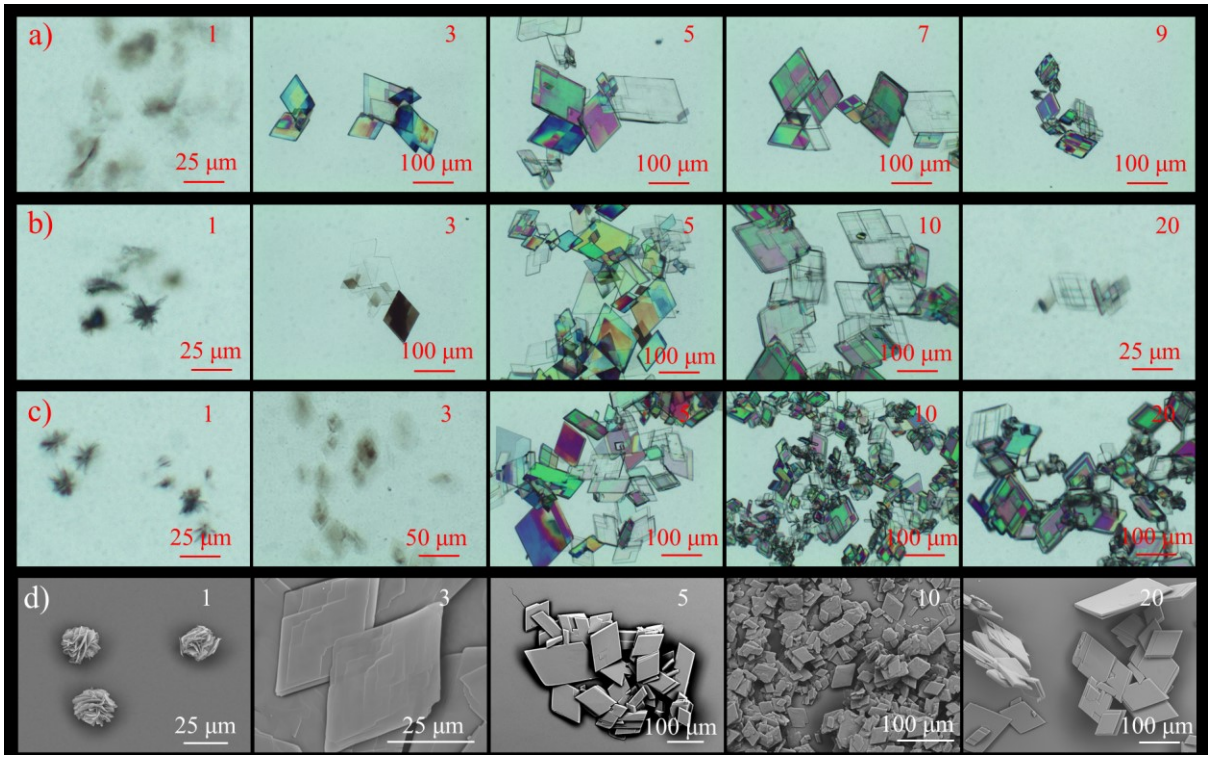

Figure S2 Optical micrograph of L-Phe with different w_o at concentration of a) 120 mM, b) 150 mM, c) 180 mM. d) SEM images of L-Phe at concentration of 180 mM. w_o is on the top right of each image.

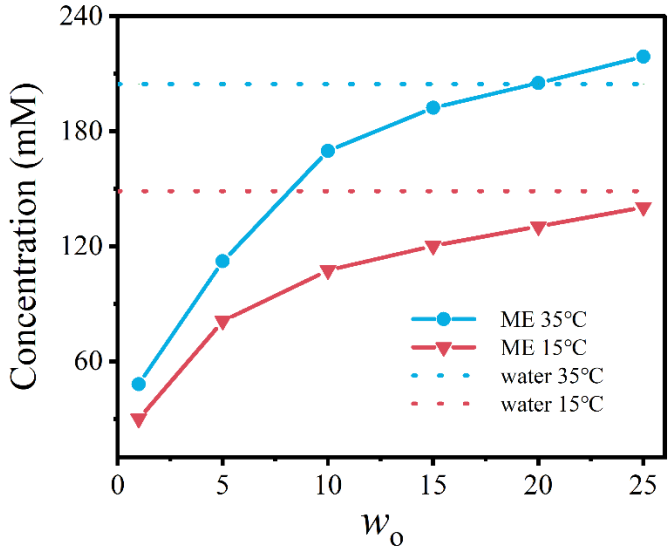

Figure S3 Solubility of L-Phe in microemulsion at 15 ℃ and 35 ℃. The dotted line represents the solubility of L-Phe in pure water, and the solid line represents the ratio of L-Phe in water of ME.

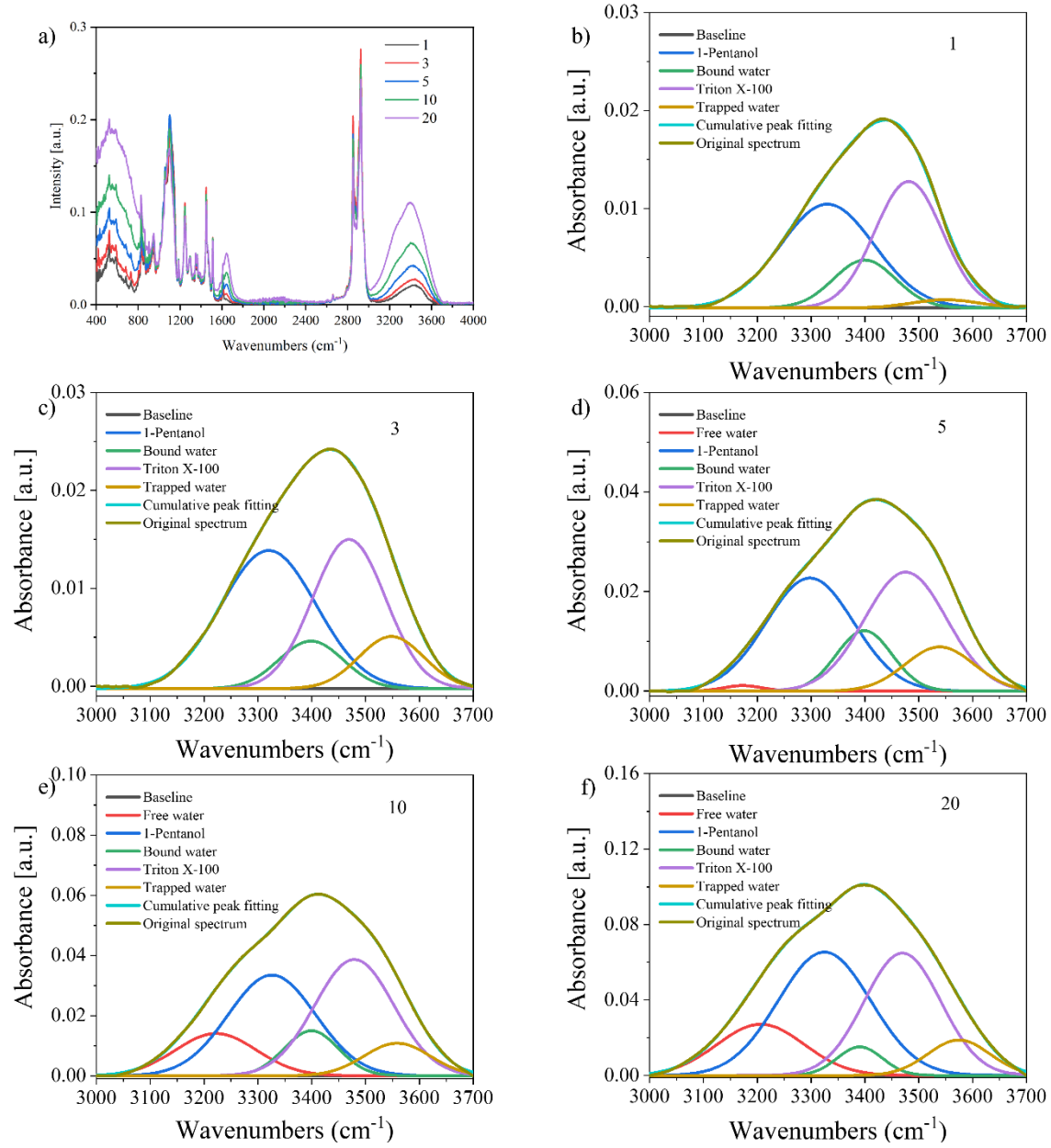

Figure S4 a) ATR-FTIR spectra of ME (w_o = 1, 3, 5, 10, 20). b-f) The O–H stretching region (3000–3700 cm^{-1}) of ME in all systems were fitted with a Gaussian program in OriginLab software, the fitting peaks correspond to free water (3200 ± 20), 1-pentanol (3310 ± 10), bound water (3395 ± 10), Triton X-100 (3470 ± 10), trapped water (3555 ± 10), respectively.

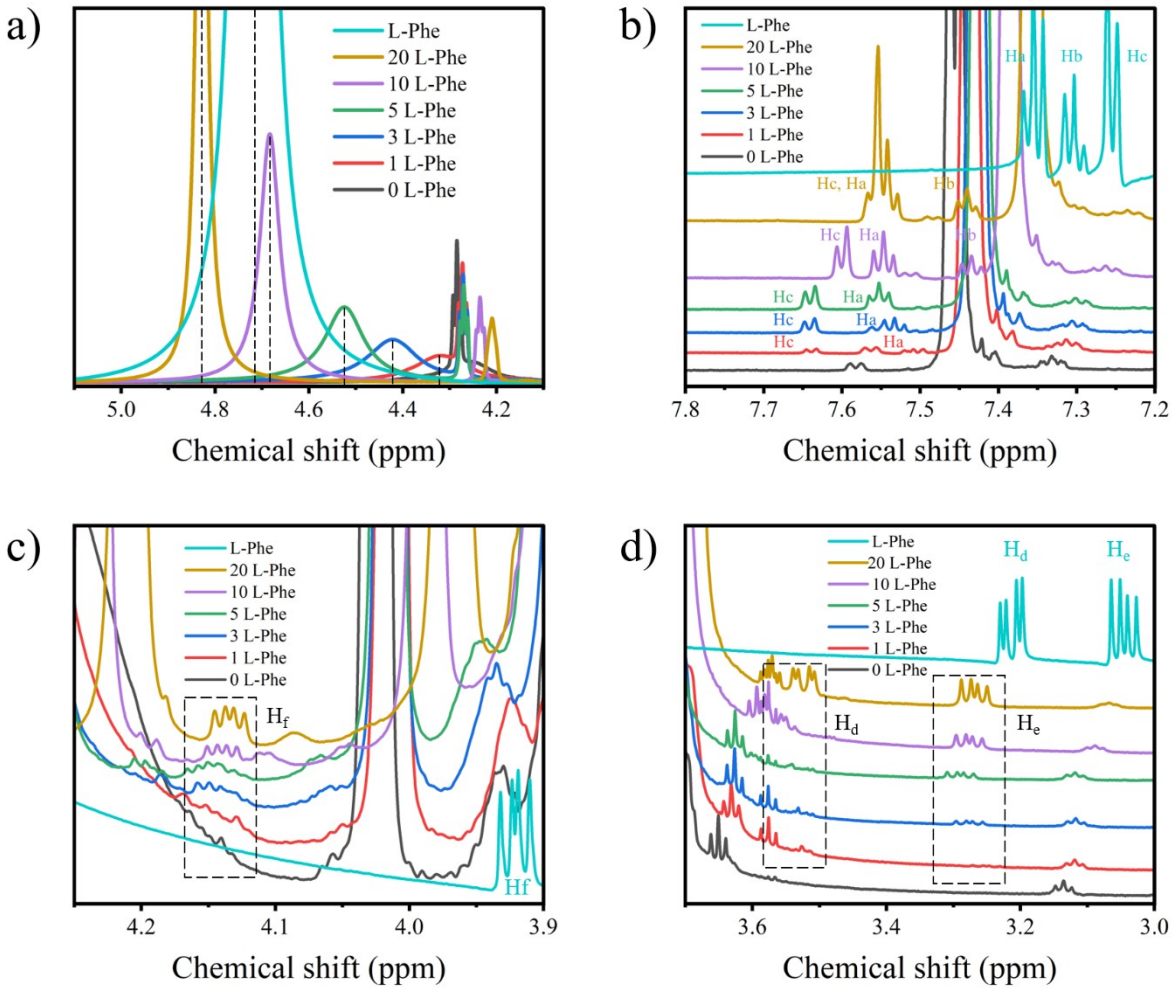

Figure S5 ^{1}H NMR profiles of L-Phe in microemulsion. Partial enlarged drawing in Figure 4a corresponds to a) ^{1}H of water, b) H_a, H_b, H_c of L-Phe, c) H_f of L-Phe, d) H_d of L-Phe.

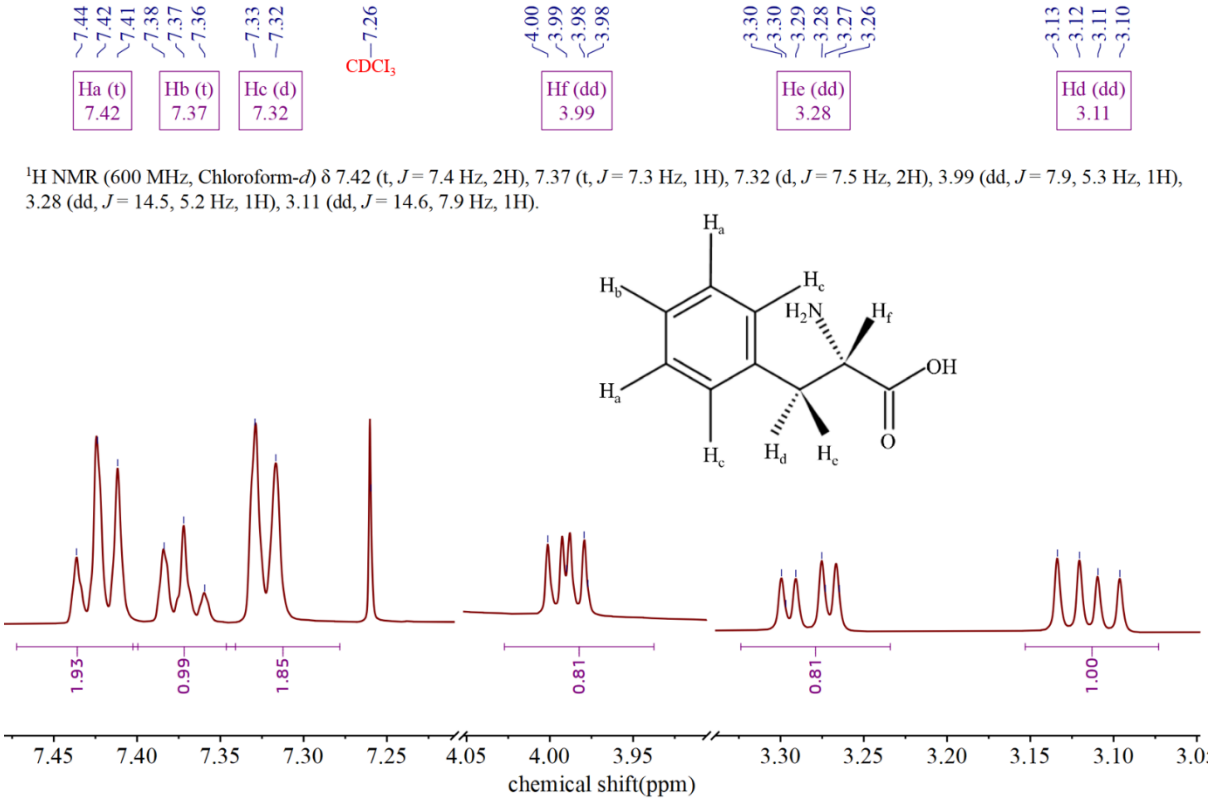

Figure S6 NMR profiles of L-Phe in bulk solution. ^{1}H (600 MHz; $CDCl_3$) NMR spectrum of L-phenylalanine. δ 7.42 (t, J = 7.4 Hz, 2H), 7.37 (t, J = 7.3 Hz, 1H), 7.32 (d, J = 7.5 Hz, 2H), 3.99 (dd, J = 7.9, 5.3 Hz, 1H), 3.28 (dd, J = 14.5, 5.2 Hz, 1H), 3.11 (dd, J = 14.6, 7.9 Hz, 1H).

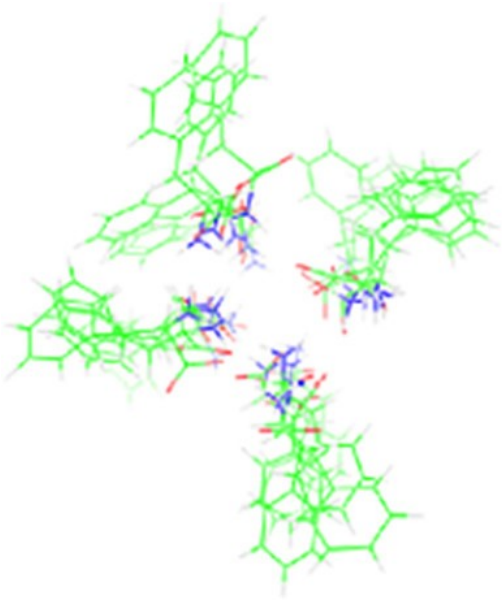

Figure S7 Proposed lowest energy structure of L-phenylalanine. Copyright © 2015, American Chemical Society.

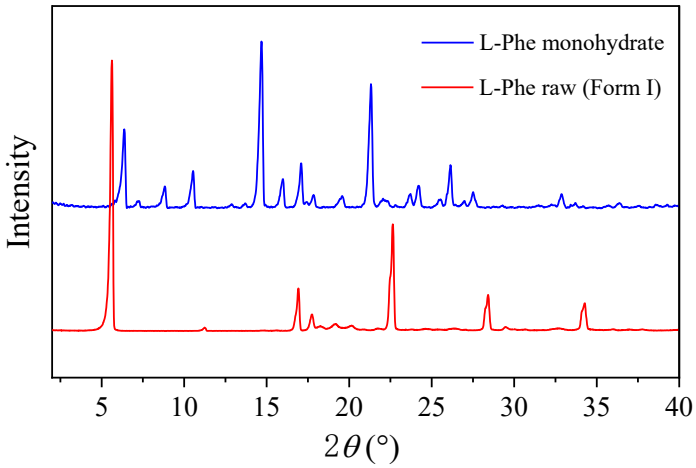

Figure S8 XRD of L-Phe. Red line is the prepared L-Phe monohydrate sample, blue line is raw of L-Phe (form I).