Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Understanding the self-ordering of amino acids into supramolecular architects: Co-assembly based modulation of phenylalanine nanofibrils

Prabhjot Singh[a], Satish K. Pandey[b], Aarzoo Grover[†,c], Rohit K. Sharma[c] and Nishima Wangoo[d,*]

[a]*Centre for Nanoscience and Nanotechnology, Panjab University, Sector 25, Chandigarh-160014, India.*

[b]*Central Scientific Instruments Organization, Sector-30C, Chandigarh-160030, India.*

[c]*Department of Chemistry & Centre for Advanced Studies in Chemistry, Panjab University, Sector 14, Chandigarh-160014, India.*

[d]*Department of Applied Sciences, University Institute of Engineering and Technology (U.I.E.T.), Panjab University, Chandigarh-160014, India.*

*E-mail: - nishima@pu.ac.in

Present Address

[†]Department of Chemistry, University of Vermont, Burlington, Vermont-05405, USA.

Table S1. Amino potential value, hydrophobicity index (kyte doolitte and GES), and solubility profile in water for amino acids divided into separate categories

Amino Acid		Hydration potential value	Hydrophobicity Index (Kyte Doolittle)	Hydrophobicity Index (GES)	Solubility in water (mg/mL)
Category I					
Amino acids with neutral aliphatic side chain (except glycine and proline)	Glycine	2.39	-0.4	1.0	250
	leucine	2.28	3.8	2.8	24
	Isoleucine	2.15	4.5	3.1	34
	Valine	1.99	4.2	2.6	88
	Alanine	1.94	1.8	1.6	166
	Cysteine	-1.24	2.5	2.0	277
	Methionine	-1.48	1.9	3.4	33
	Proline	-	-1.6	-0.2	1620
Category II					
Amino acids with hydroxyl group in the side chain	Threonine	-4.88	-0.7	1.2	97
	Serine	-5.06	-0.8	0.6	425
Category III					
Amino acids with amide group in the side chain	Glutamine	-9.38	-3.5	-4.1	41.3
	Asparagine	-9.68	-3.5	-4.8	29.4
Category IV					
Amino acids with carboxylic group in the side chain	Glutamic acid	-10.20	-3.5	-8.2	8.5
	Aspartic acid	-10.95	-3.5	-9.2	5.3
Category V					
Amino acid with cationic side chain	Lysine	-9.52	-3.9	-8.8	1000
	Histidine	-10.27	-3.2	-3.0	45
	Arginine	-19.92	-4.5	-12.3	182

Table S2: - Various set of conditions for the geenration of amino acid self assembled structures

Category	Amino Acid	Water Solubility (mg/mL)	Condition (Concentration, solvent)	Morphology
Category I	Glycine	249.0	1 mg/mL, Water and **water:methanol (1:1)**	MIcro crystallite arranged in Fern Structure
	Alanine	166.0	1 mg/mL, Water and **water:methanol (1:1)**	Micro crystallite arranged in Fern Structure
	Leucine	24.2	1 mg/mL, Water and **water:methanol (1:1)**	Micro crystallite arranged in Fern Structure
	Isoleucine	41.1	1 mg/mL, Water and **water:methanol (1:1)**	Micro crystallite arranged in Fern Structure
	Valine	58.5	1 mg/mL, **Water** and water:methanol (1:1)	Micro crystallite deposits
	Proline	1623.0	5 mg/mL, **80% methanol in water**	Crystallite Micro rod
	Methionine	33.8	1 mg/mL, Water and **water:methanol (1:1)**	Micro crystallite arranged in Fern Structure
	Cysteine	277.0	1 mg/mL, Water and **water:methanol (1:1)**	**Globular** and elongated needle like
Category II	Serine	425.0	Water and **water:methanol (1:1) at each 50^{0}C evaporation temperature**	Micro Capsule shape
	Threonine	97.0	1 mg/mL, **water**	Micro Spear
Category III	Asparagine	29.4	1 mg/mL, Water and **water:methanol (1:1)**	Micro Floral dendritic
	Glutamine	41.3	1 mg/mL, **water:methanol (1:1)**	Micro Floral dendritic
Category IV	Glutamic acid	8.5	1 mg/mL, **water**	Membrane like
	Aspartic acid	5.4	1 mg/mL, Aqueous ammonia (0.1M)	Membrane like
Category V	Lysine	1000.0	1 mg/mL, 0.1 M aqueous NaOH	Crystalline rod
	Arginine	182	1 mg/mL, 0.1 M aqueous NaOH	Crystalline needle
	Histidine	45.6	1 mg/mL, water:methanol (1:1), **aqueous pH 8.0 in methanol:water**	Micro fibril

Category I

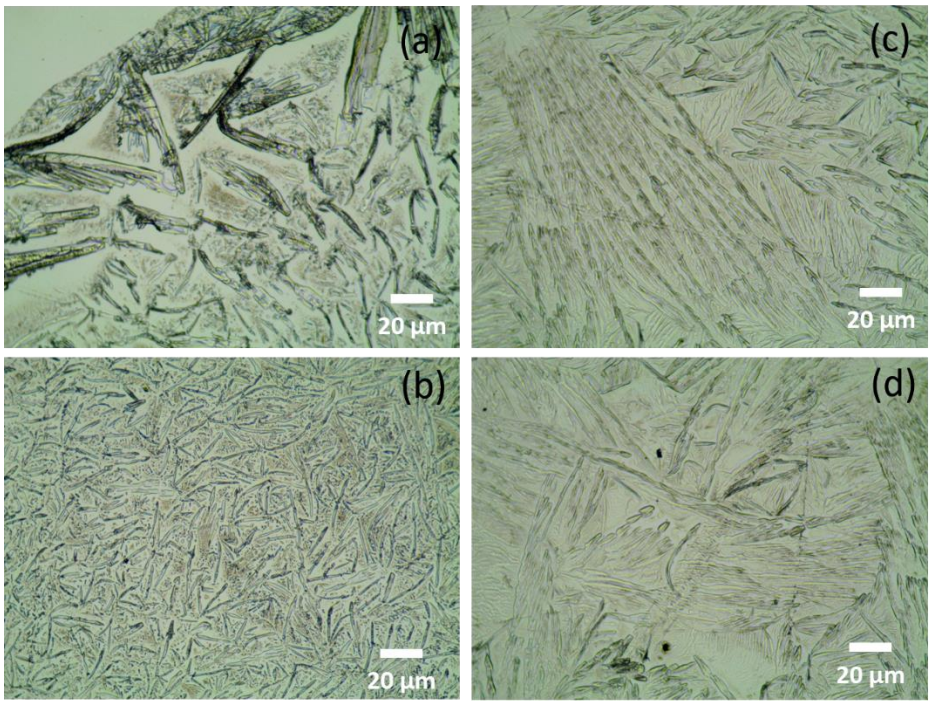

Figure S1a: - Optical microscopy images for self assembly of glycine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

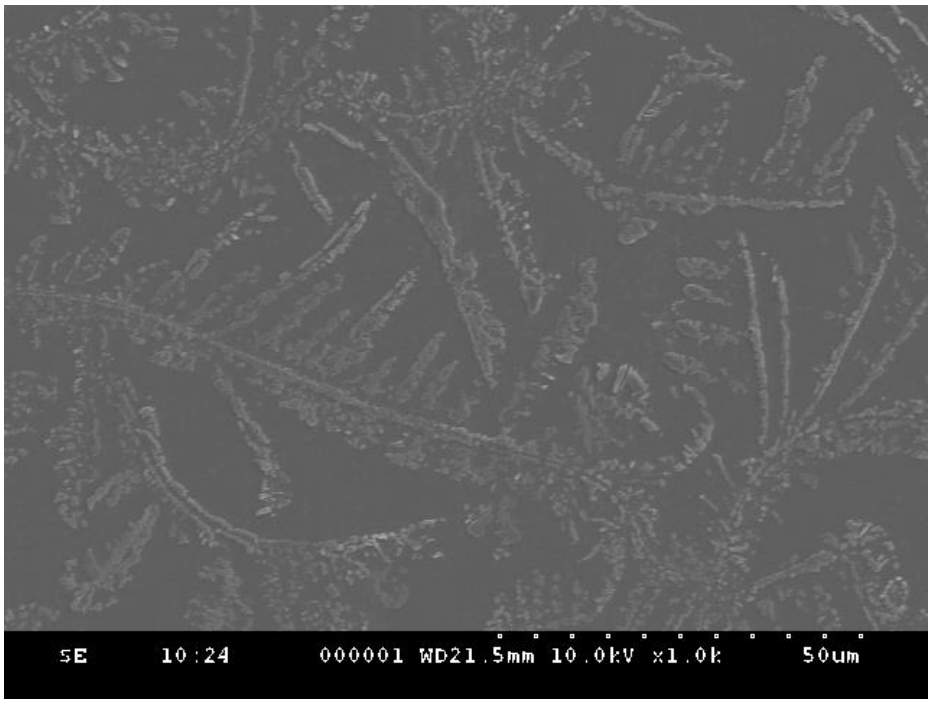

Figure S1b: - FESEM image for self assembly of glycine in water methanol (1:1) solvent system at 1 mg/mL concentration

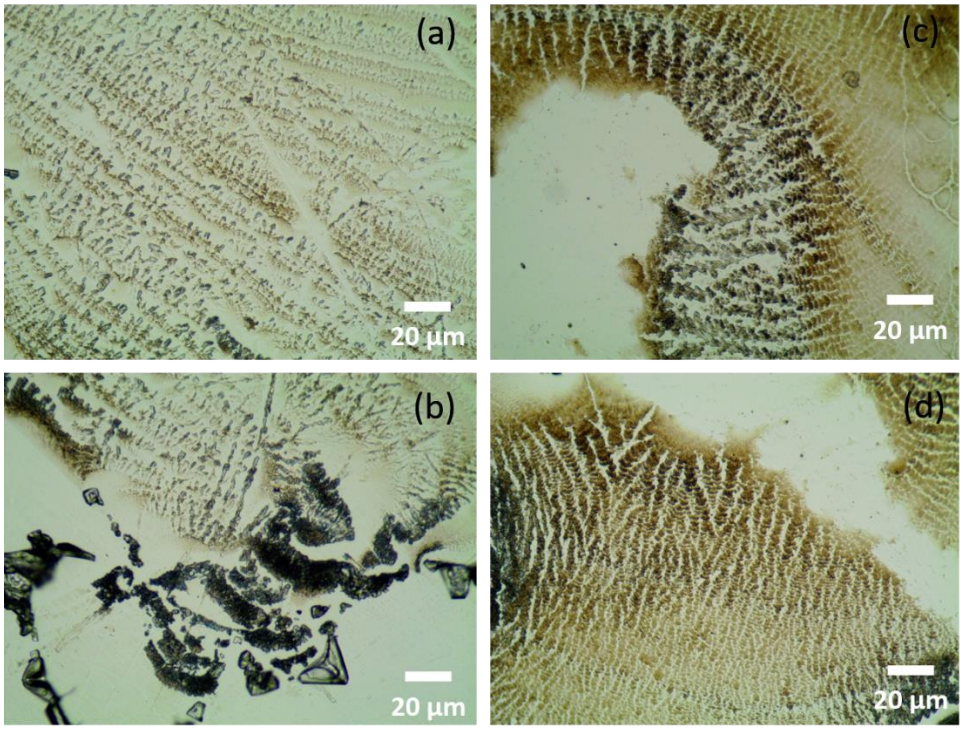

Figure S2a: - Optical microscopy images for self assembly of alanine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

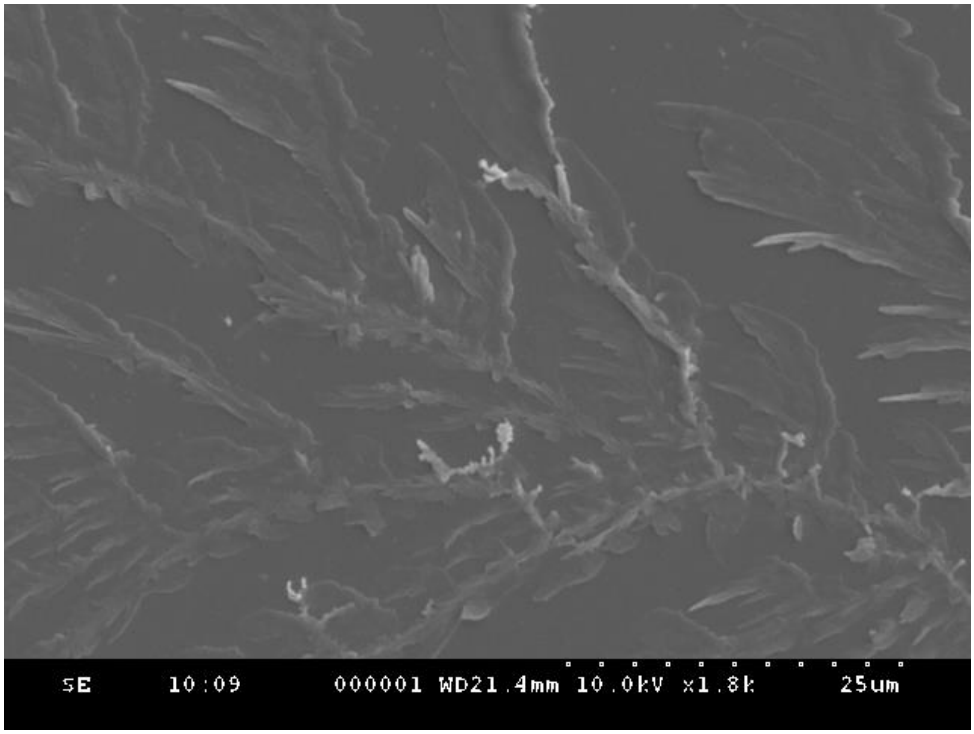

Figure S2b: - FESEM image for self assembly of alanine in water methanol (1:1) solvent system at 1 mg/mL concentration

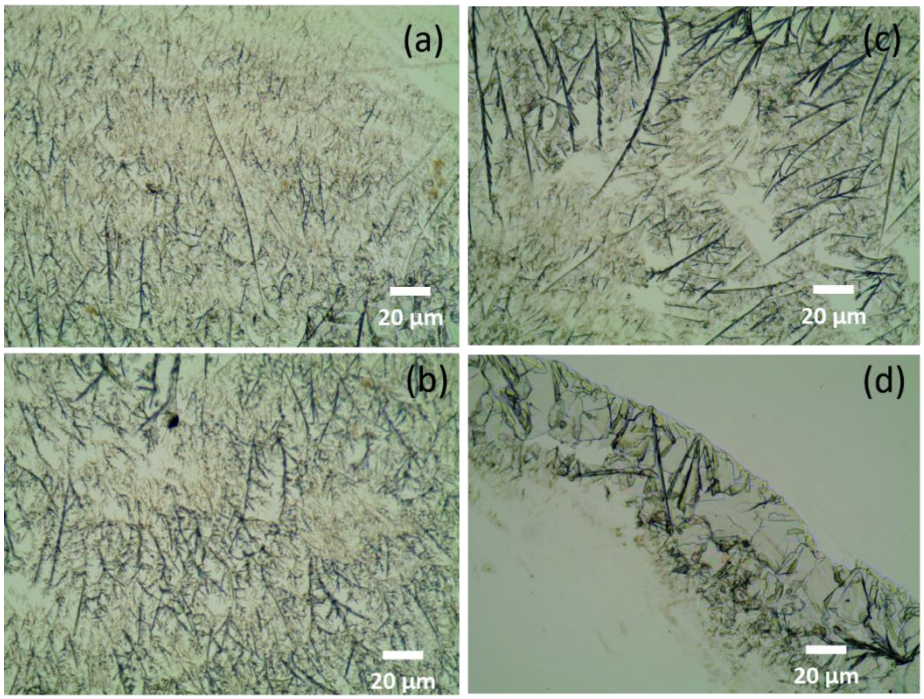

Figure S3a: - Optical microscopy images for self assembly of leucine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

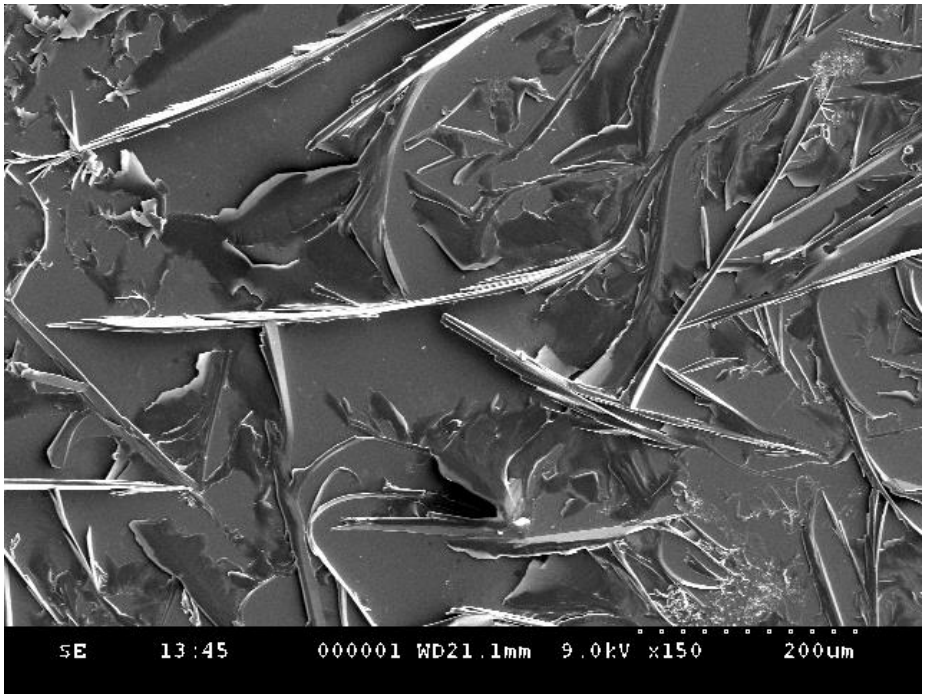

Figure S3b: - FESEM image for self assembly of leucine in water methanol (1:1) solvent system at 1 mg/mL concentration

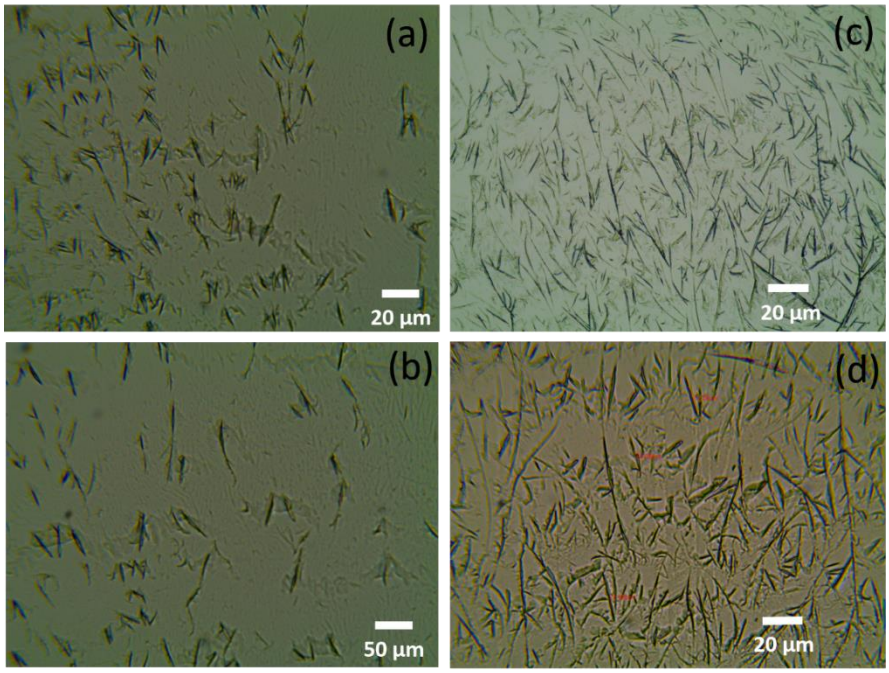

Figure S4a: - Optical microscopy images for self assembly of isoleucine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

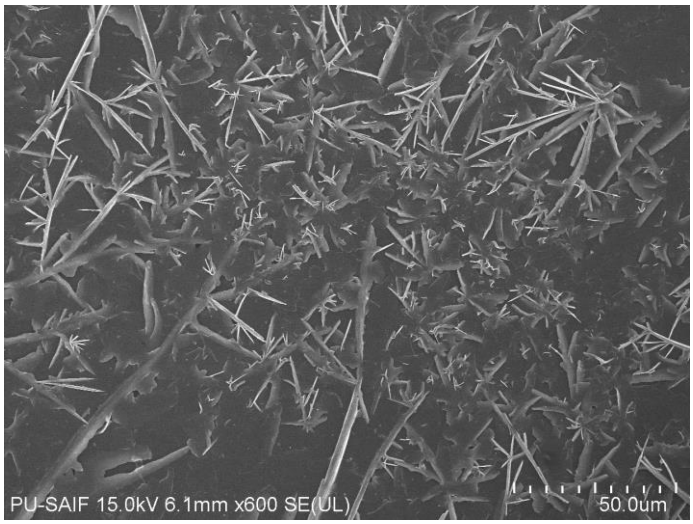

Figure S4b: - FESEM image for self assembly of isoleucine in water methanol (1:1) solvent system at 1 mg/mL concentration

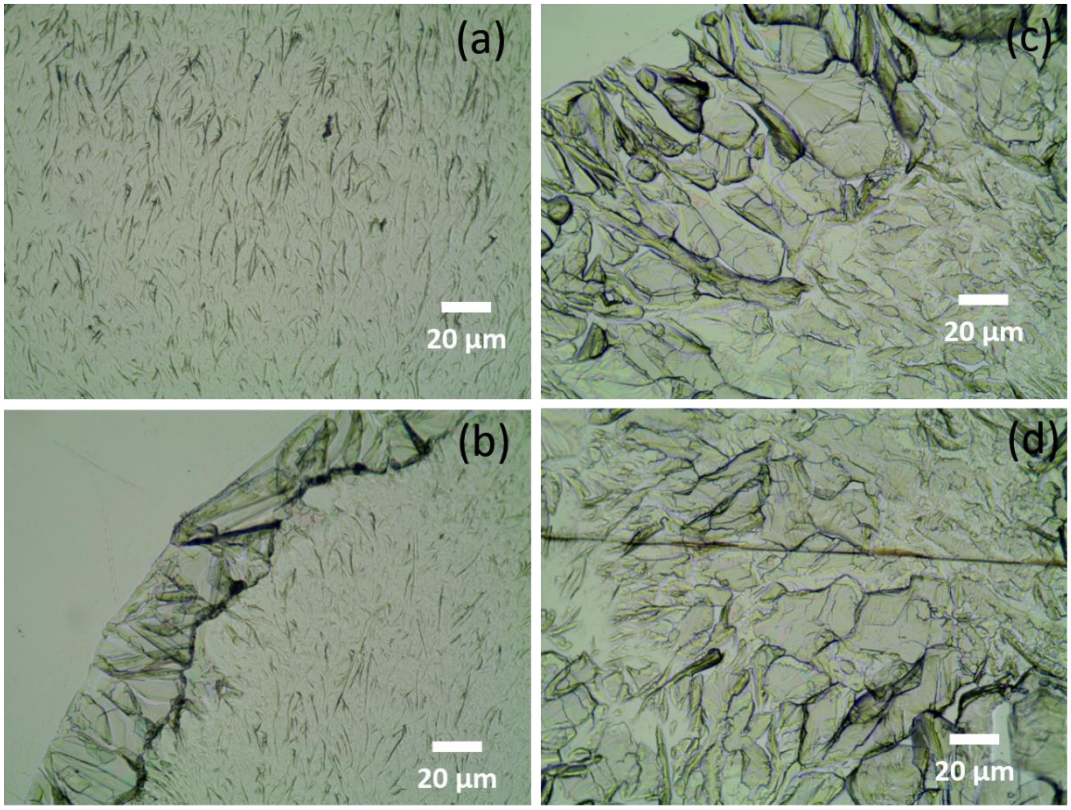

Figure S5a: Optical microscopy image for self assembly of valine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

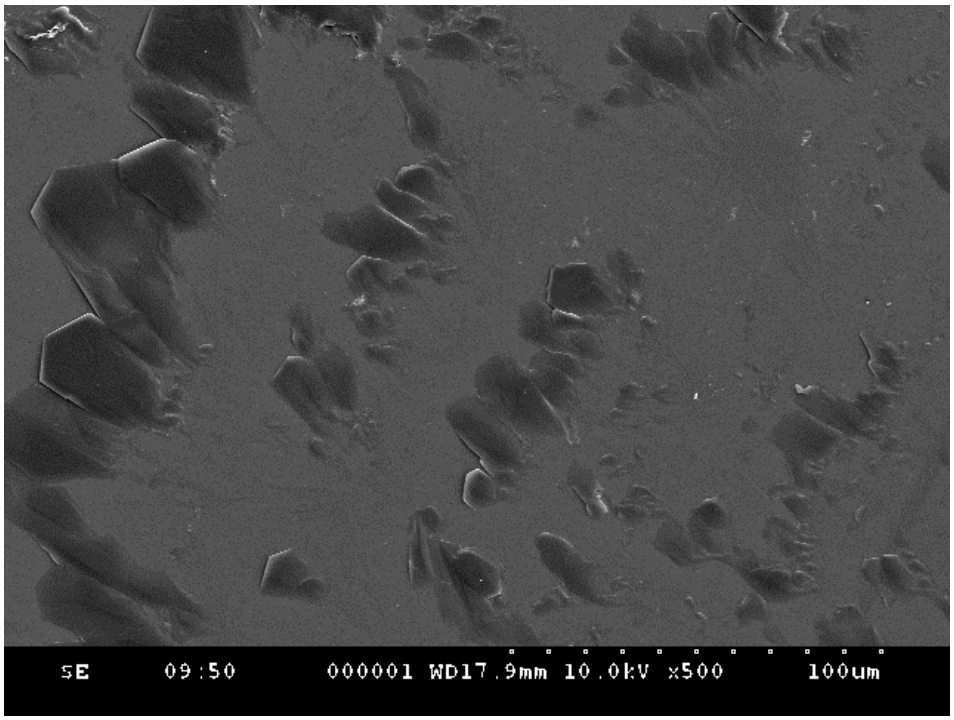

Figure S5b: - FESEM image for self assembly of valine in water at 1 mg/mL concentration

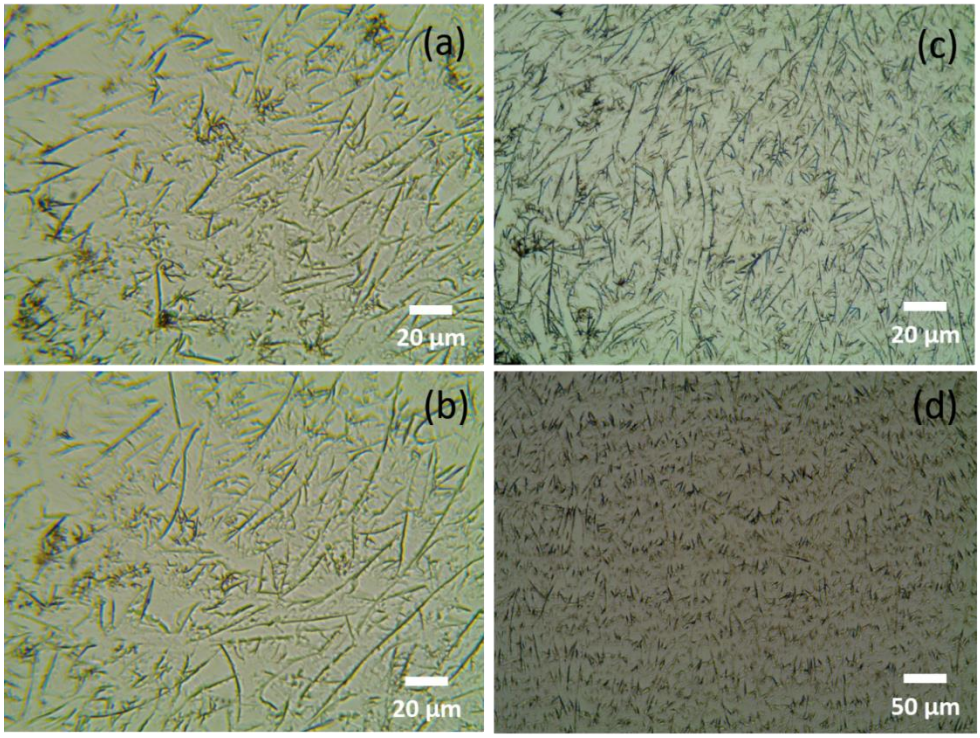

Figure S6a: - Optical microcsopy umage for self assembly of methionine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

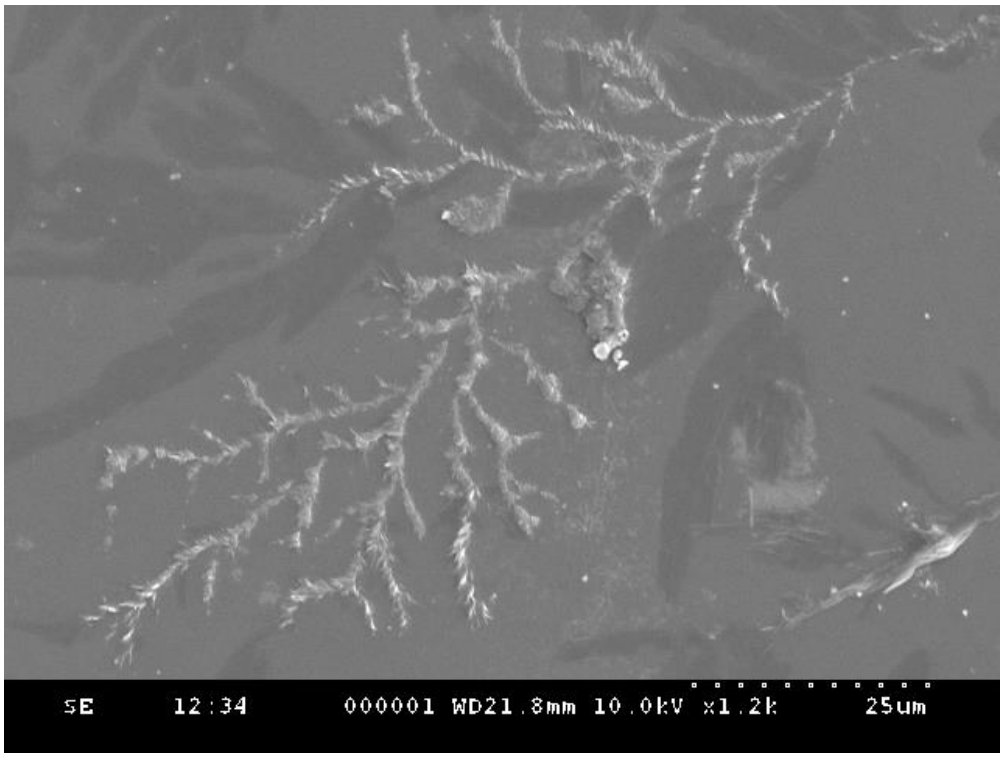

Figure S6b: - FESEM image for self assembly of methionine in water:methanol (1:1) solvent system at 1 mg/mL concentration

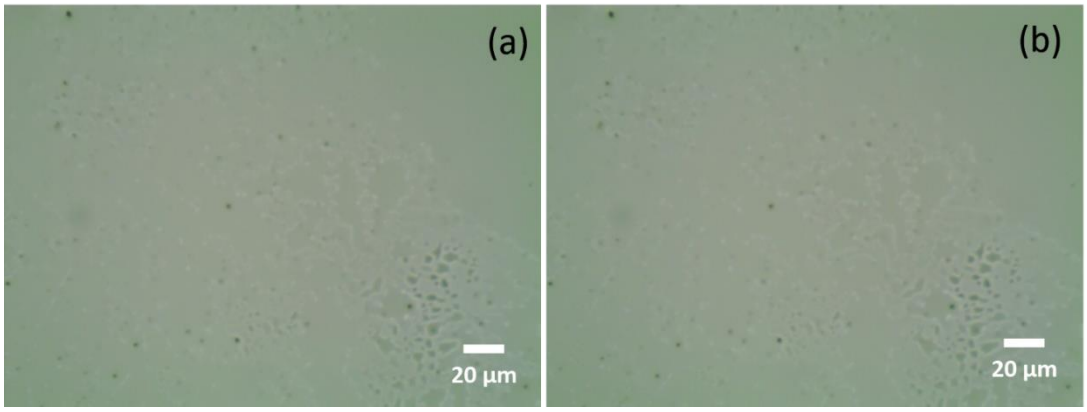

Figure S7a: Optical microscopy image for self assembly of proline in water (a) and in methanol (1:1) solvent (b) system at 1 mg/mL concentration.

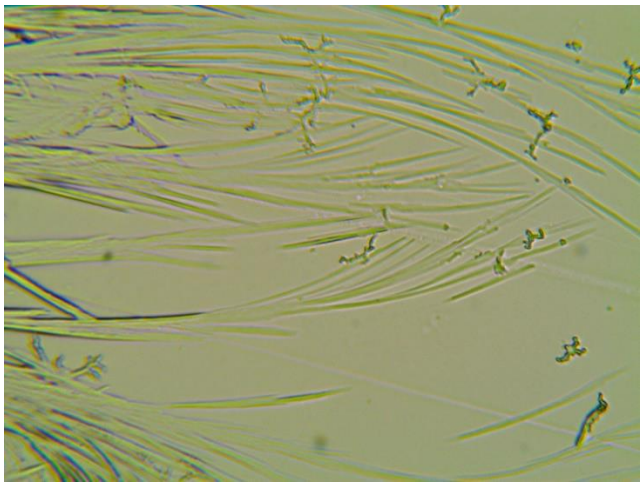

Figure S7b: Optical microscopy image for self assembly of proline in 80 % methanol in water solvent system at 5 mg/mL concentration.

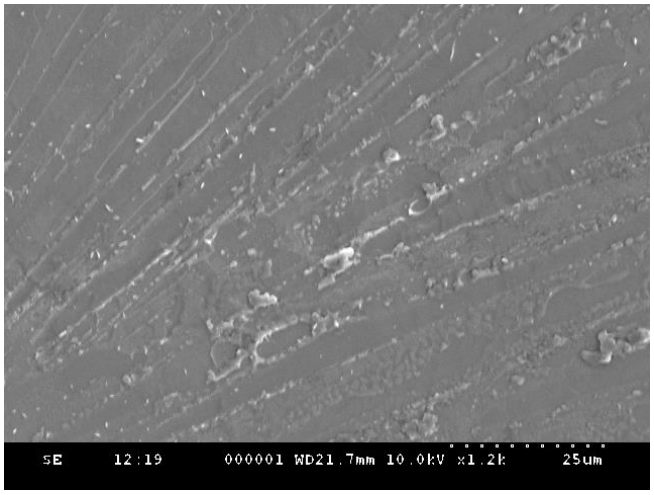

Figure S7c: - FESEM image for self assembly of proline in 80 % methanol in water solvent system at 5 mg/mL concentration.

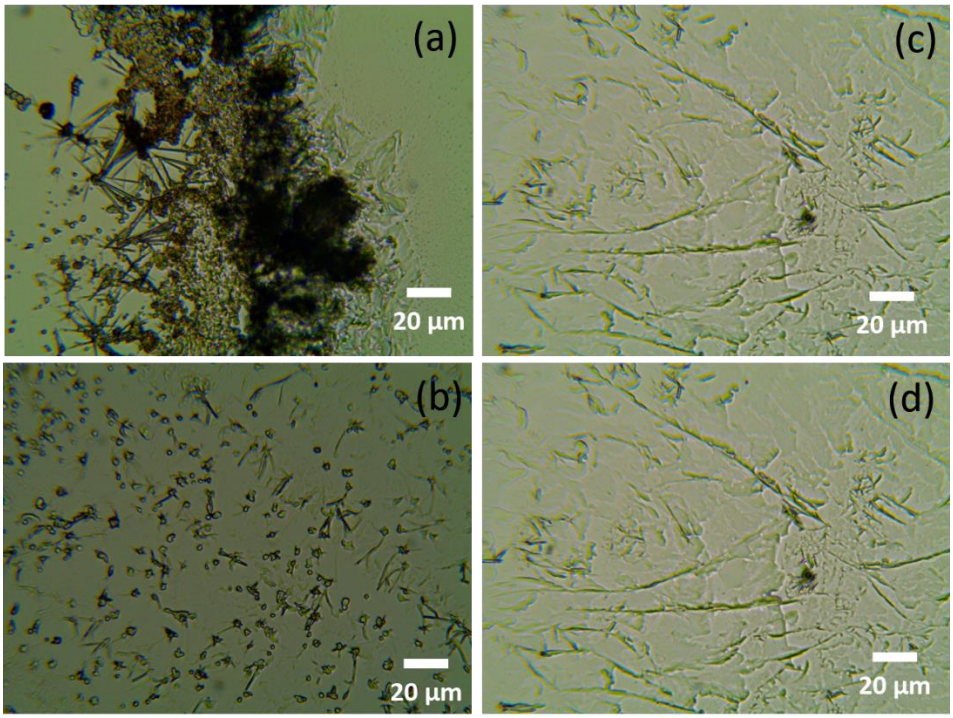

Figure S8a: Optical microscopy image for self assembly of cysteine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

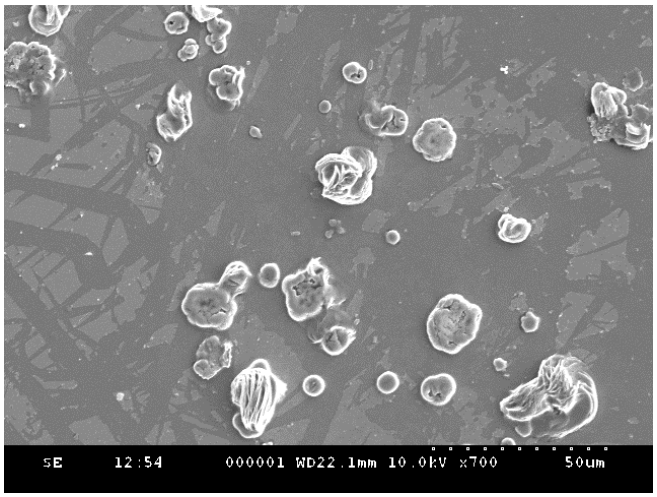

Figure S8b: FESEM image for self assembly of cysteine in water at 1 mg/mL concentration

Category II

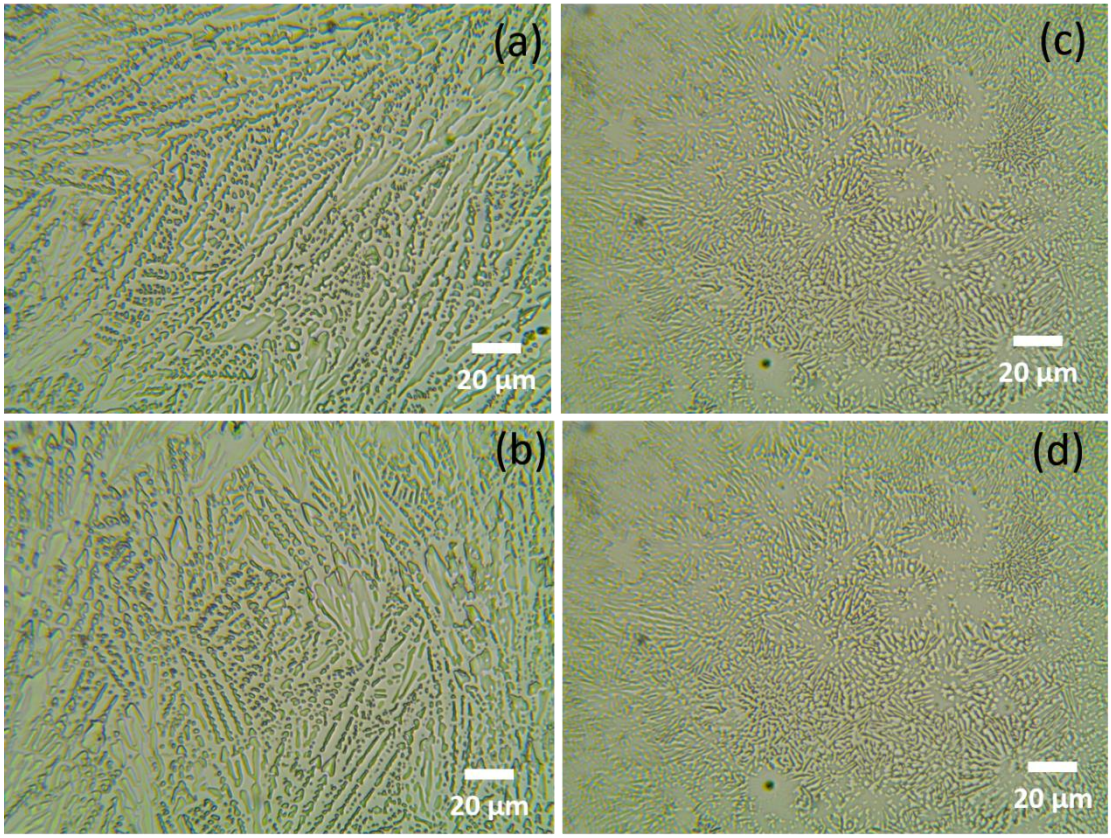

Figure S9a: - Optical images for self assembly of threonine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

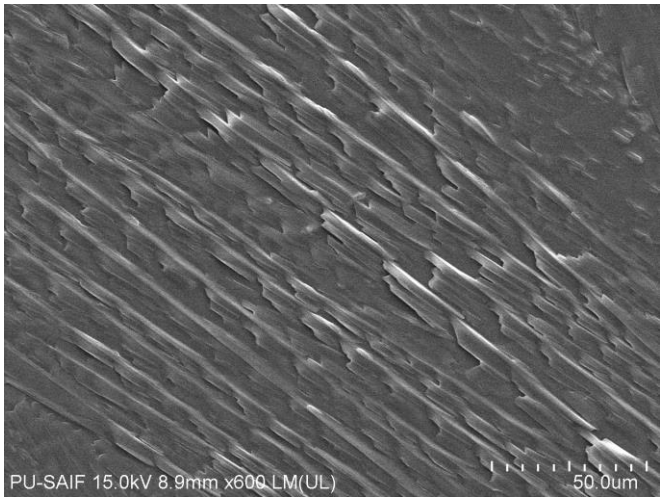

Figure S9b: - FESEM image for self assembly of threonine in water at 1 mg/mL concentration

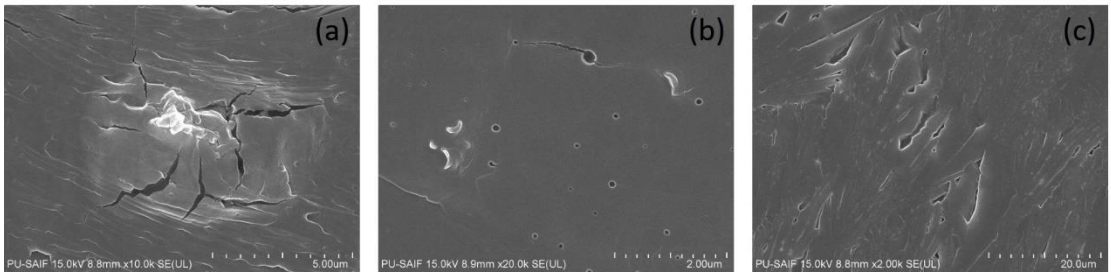

Figure S10a: - Self assembly of serine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

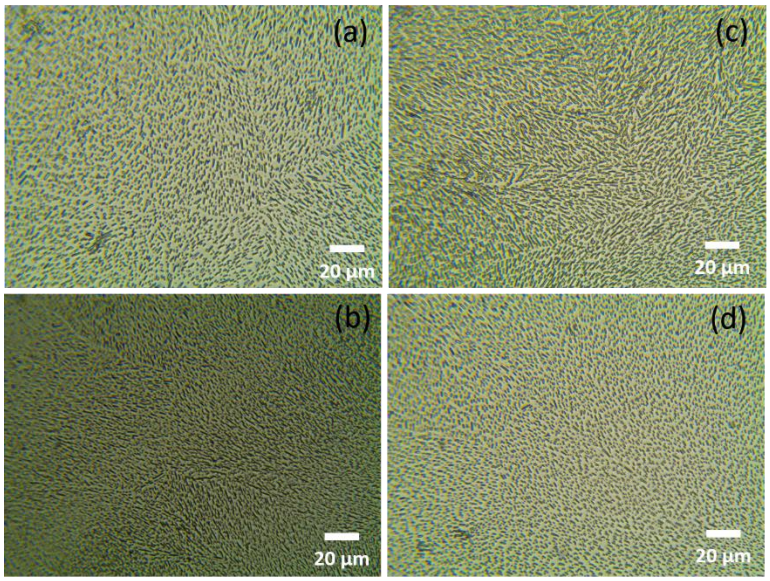

Figure S10b: - Self assembly of serine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

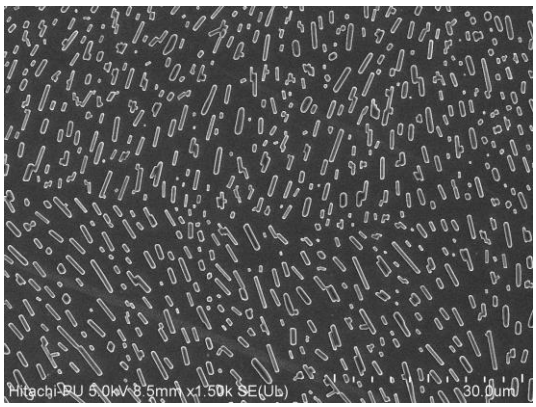

Figure S10c: - FESEM image for self assembly of serine in water at 1 mg/mL concentration

Category III

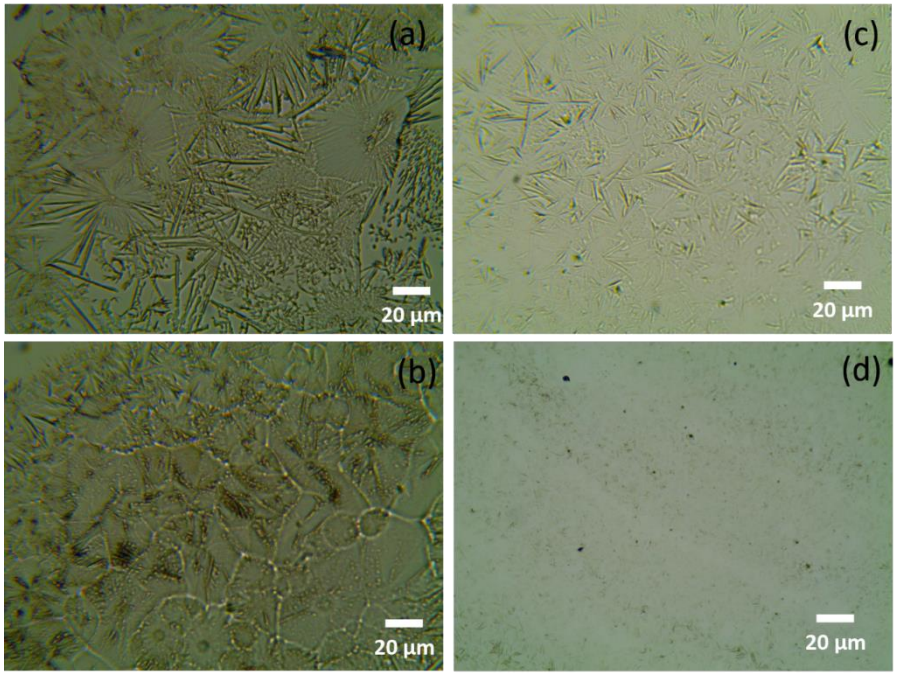

Figure S11a: - Optical images for self assembly of asparagine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

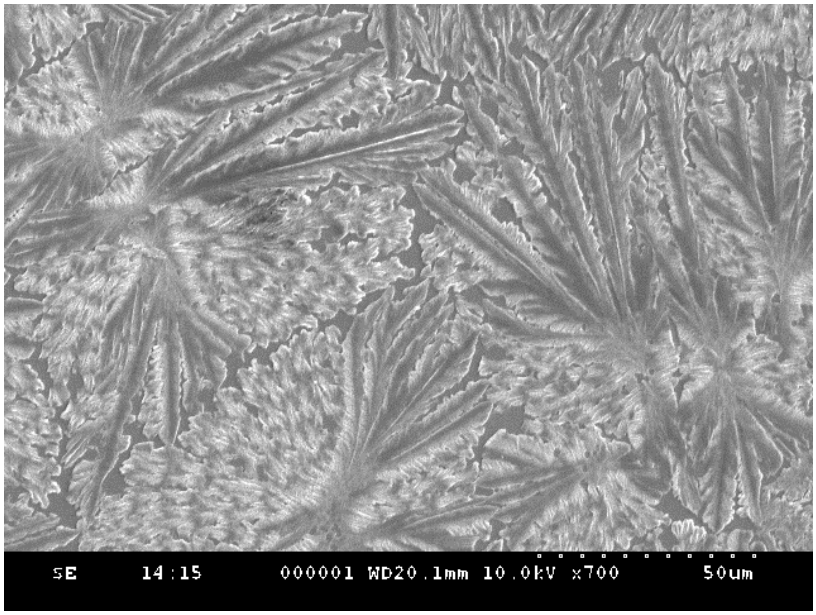

Figure S11b: - FESEM image for self assembly of asparagine in water at 1 mg/mL concentration

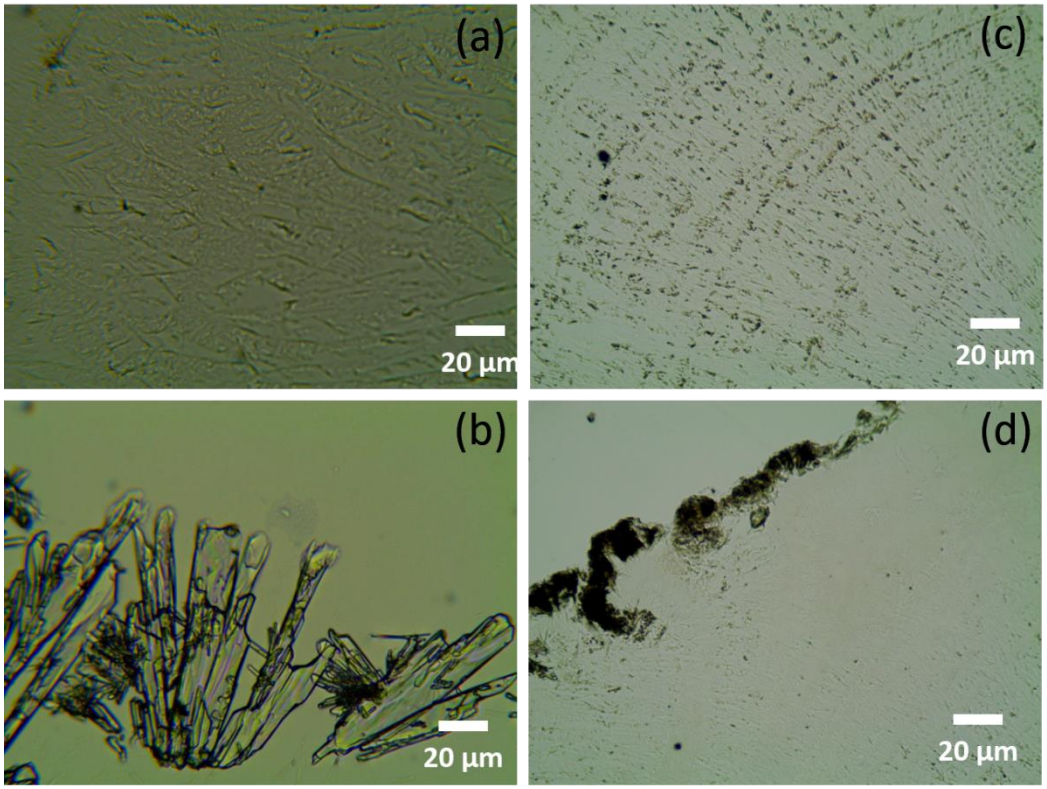

Figure S12a: - Self assembly of glutamine in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

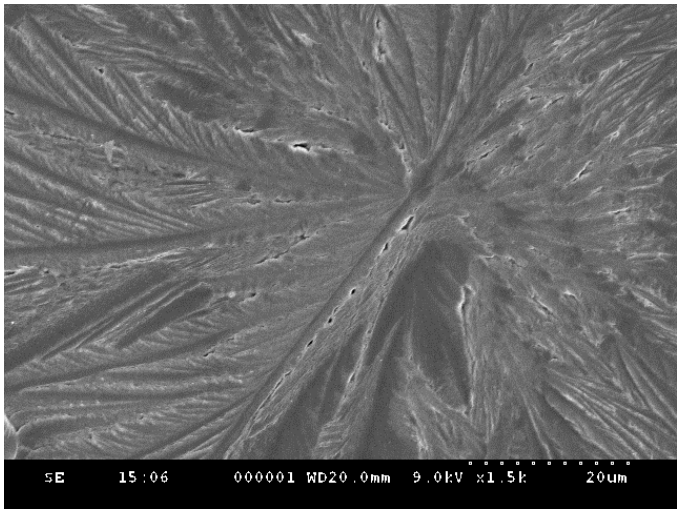

Figure S12b: - FESEM image for self assembly of glutamine in water at 1 mg/mL concentration

Category IV

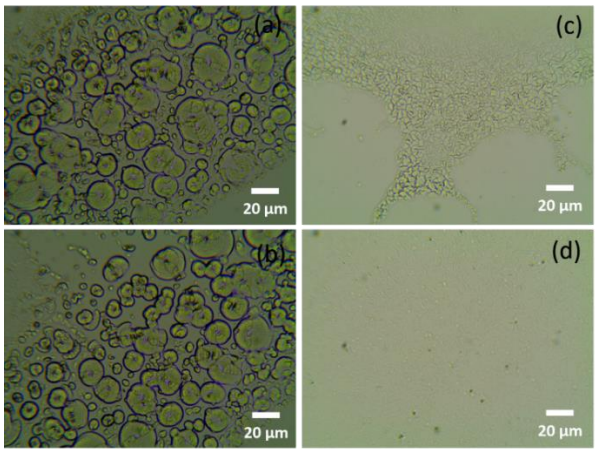

Figure S13a: - Self assembly of glutamine acid in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

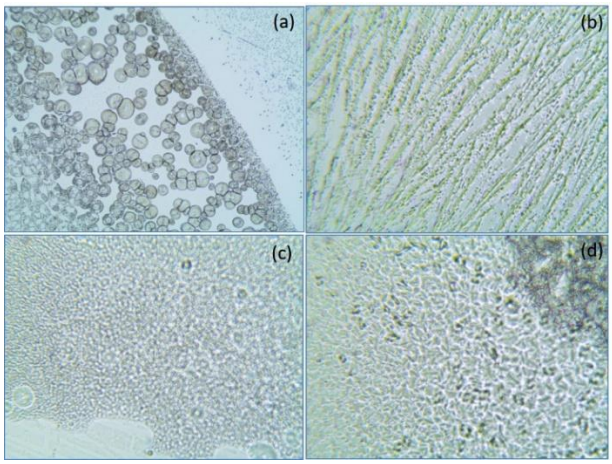

Figure S13b: - Optical microscopy images for self assembly of glutamic acid in 0.1 M HCl (a); 0.1 M NaOH (b). 0.1 M AcOH (c) and 0.1 M NH_3

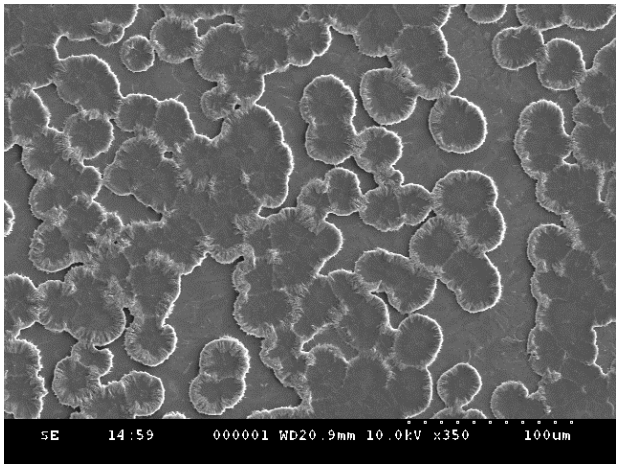

Figure S13c: - FESEM image for self assembly of glutamic acid in 0.1 M aqueous NH_3 solvent system at 1 mg/mL concentration

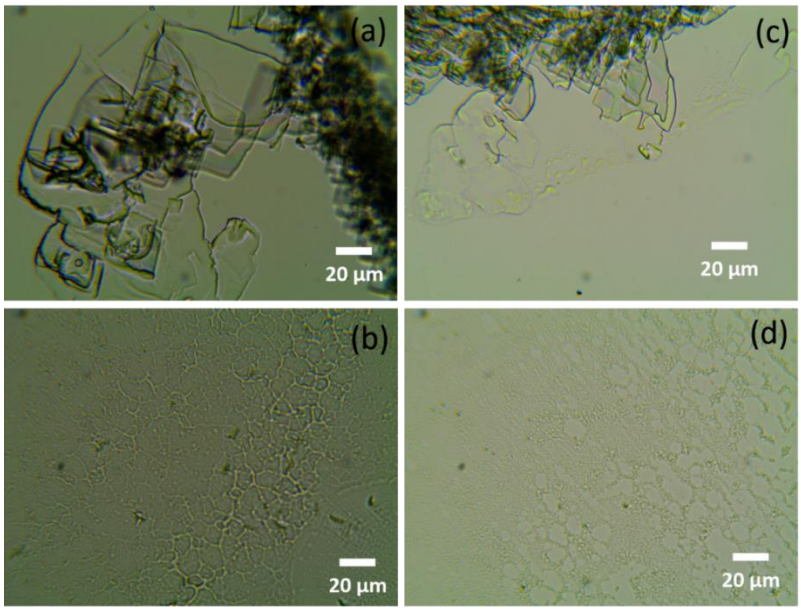

Figure S14a: - Optical images for self assembly of aspartic acid in water (a,b) and water methanol (1:1) solvent system (c,d) at 1 mg/mL concentration

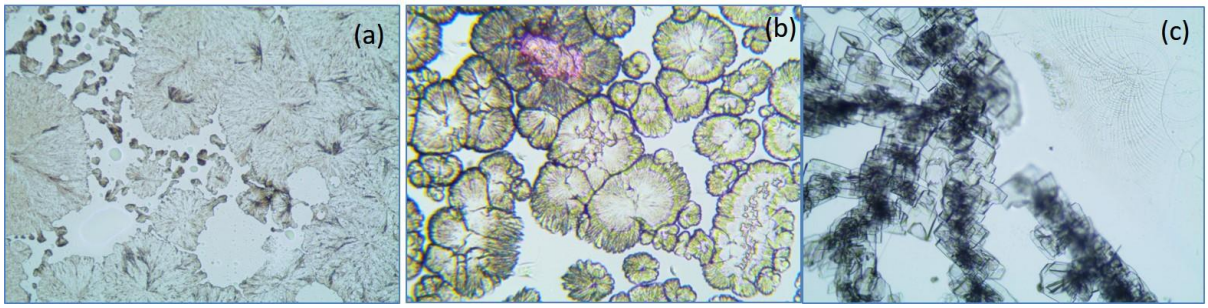

Figure 14b: - Optical microscopic images for self-assembly of aspartic acid in 0.1 M HCl (a); 0.1 M NH_3 (b); and 0.1 M AcOH.

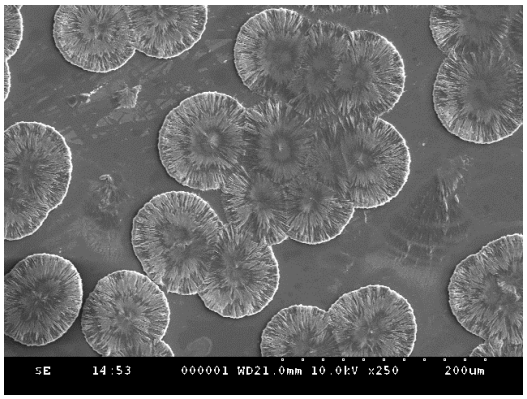

Figure 14c: - FESEM image for self-assembly of aspartic acid in 0.1 M NH_3 n aqueous medium

Category V

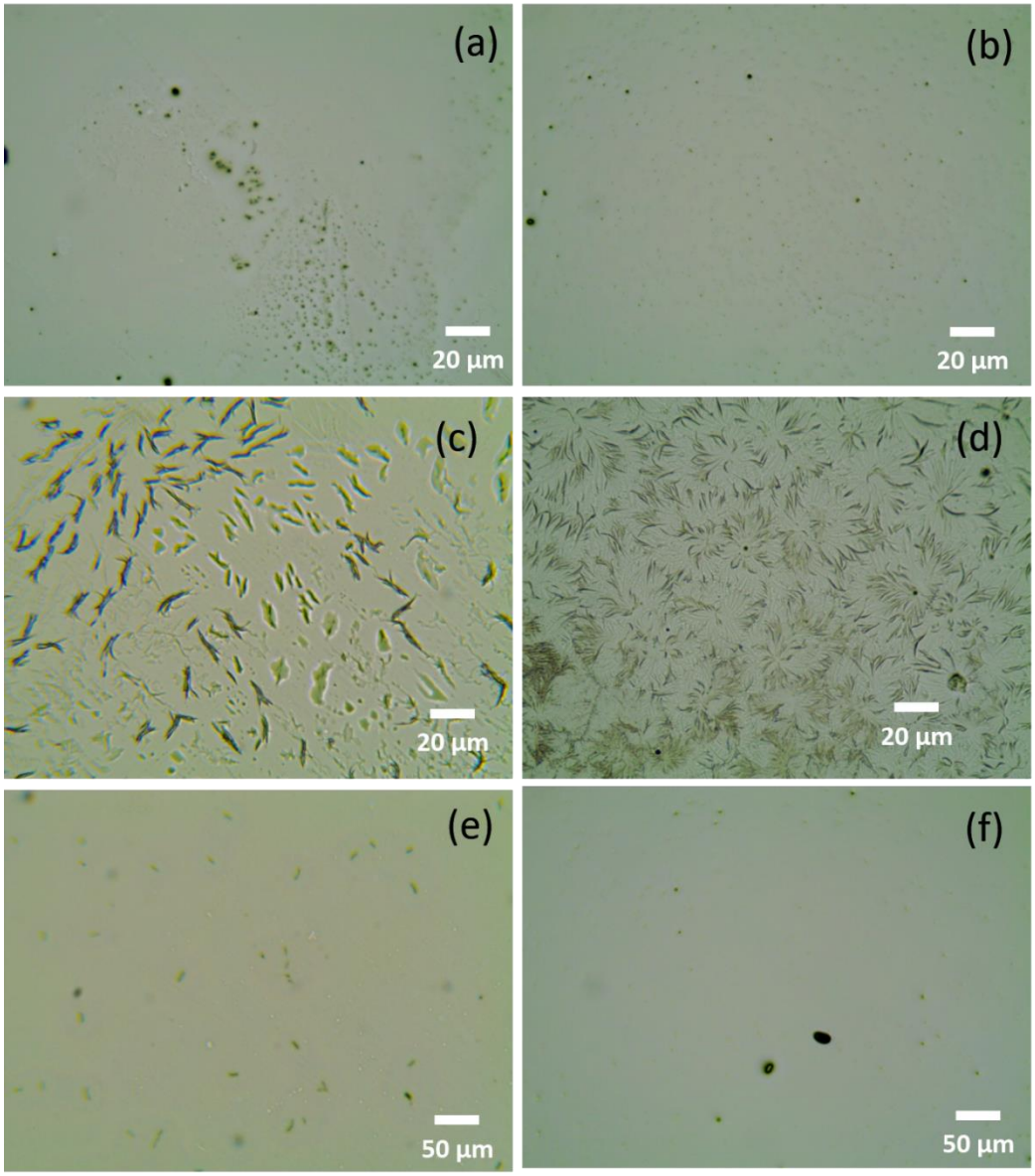

Figure S15: Self assembly of arginine, histidine and lysine in water (a, c and e, respectively) and in methanol (1:1) solvent (b, d and f, respectively) system at 1 mg/mL concentration

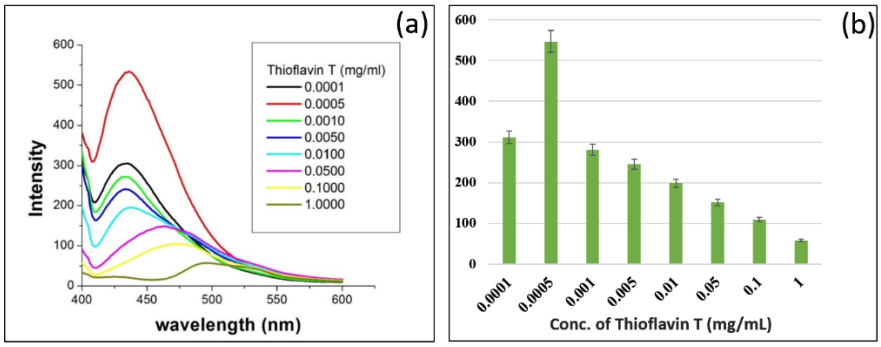

Figure S16: - Optimization of ThT concentration for maximum emission intensity in aqueous medium

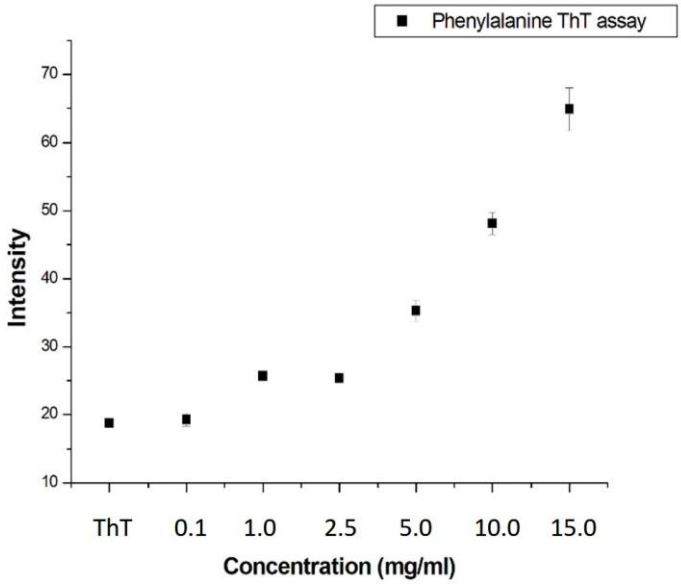

Figure S17: - Optimization of phenylalanine concentration for ThT fluorescence assay using optimized ThT concentration in aqueous medium

Phenylalanine and amino acid co-assembled structures

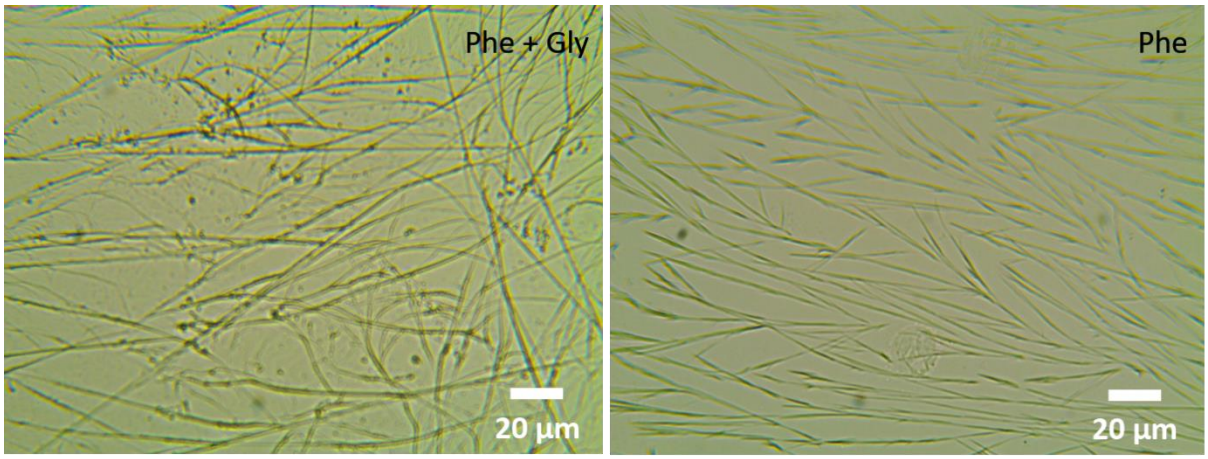

Figure S18: - Optical images for self-assembly of co-assembled phenylalanine:glycine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

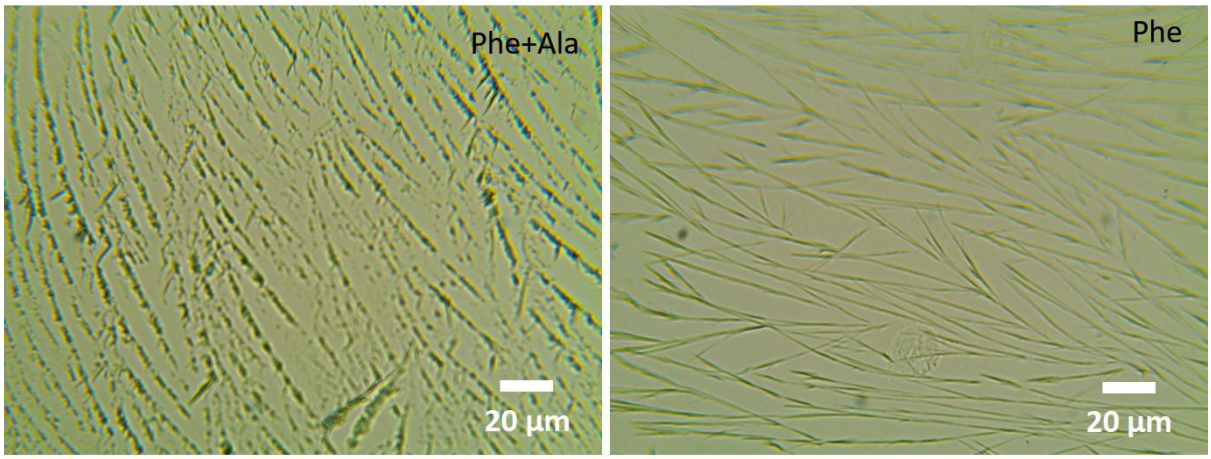

Figure S19: - Optical images for self-assembly of co-assembled phenylalanine:alanine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

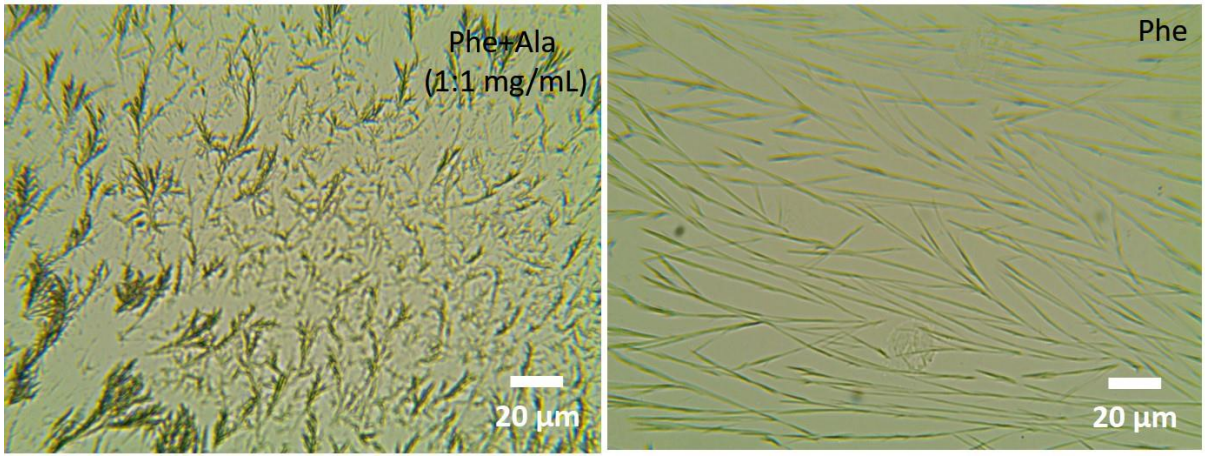

Figure S20: - Optical images for self-assembly of co-assembled phenylalanine:alanine (1mg/mL and 1 mg/mL, respectively) and only phenylalanine in aqueous medium

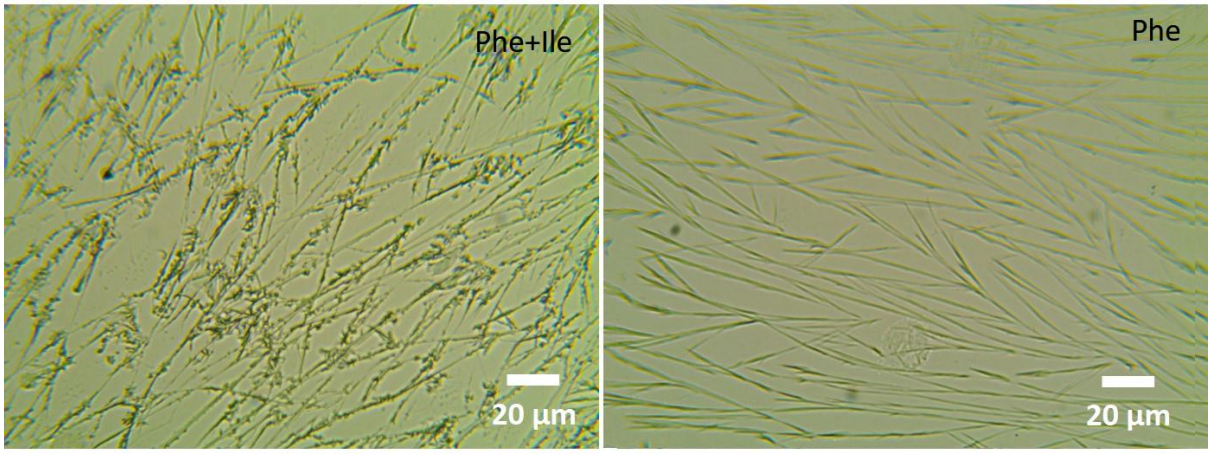

Figure S21: - Optical images for self-assembly of co-assembled phenylalanine:isoleucine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

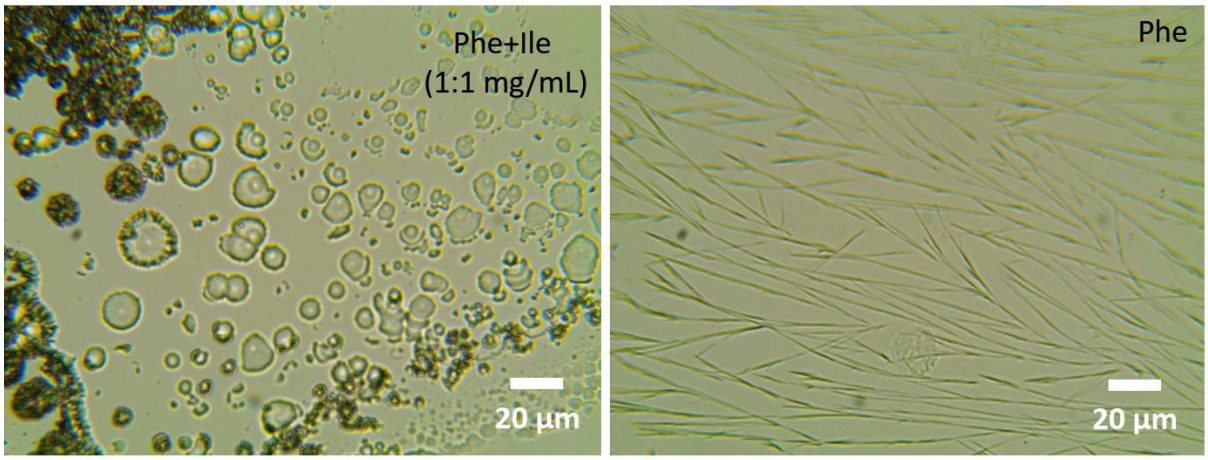

Figure S22: - Optical images for self-assembly of co-assembled phenylalanine:isoleucine (1mg/mL and 1 mg/mL, respectively) and only phenylalanine in aqueous medium

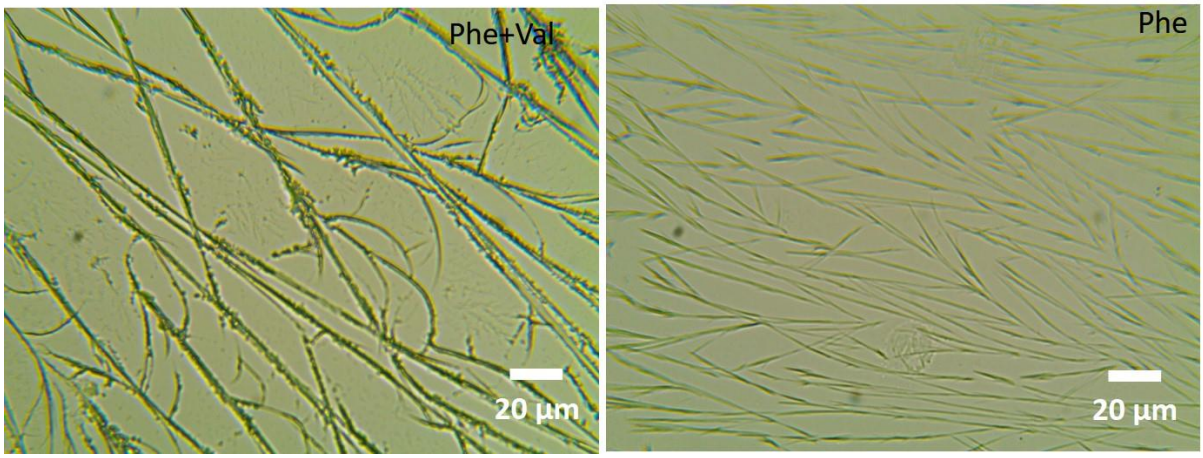

Figure S23: - Optical images for self-assembly of co-assembled phenylalanine:valine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

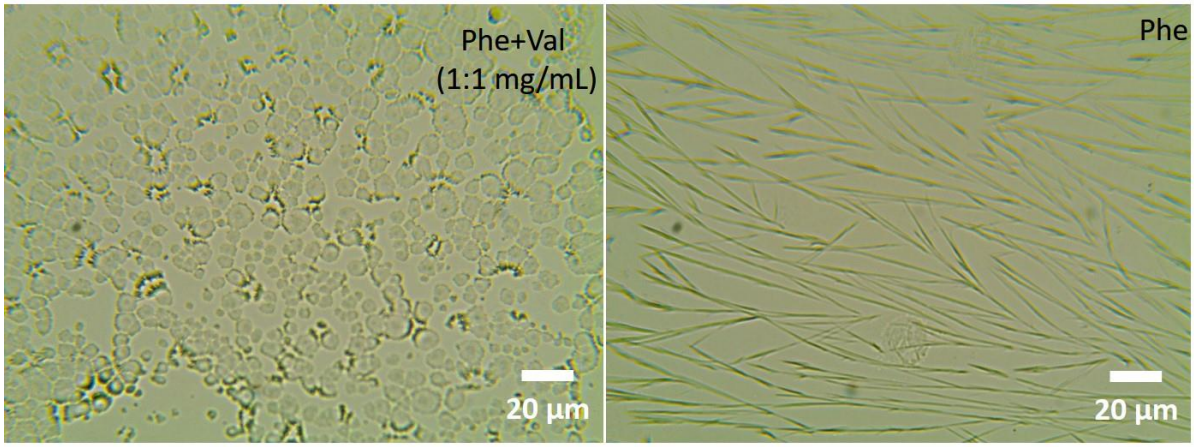

Figure S24: - Optical images for self-assembly of co-assembled phenylalanine:valine (1mg/mL and 1 mg/mL, respectively) and only phenylalanine in aqueous medium

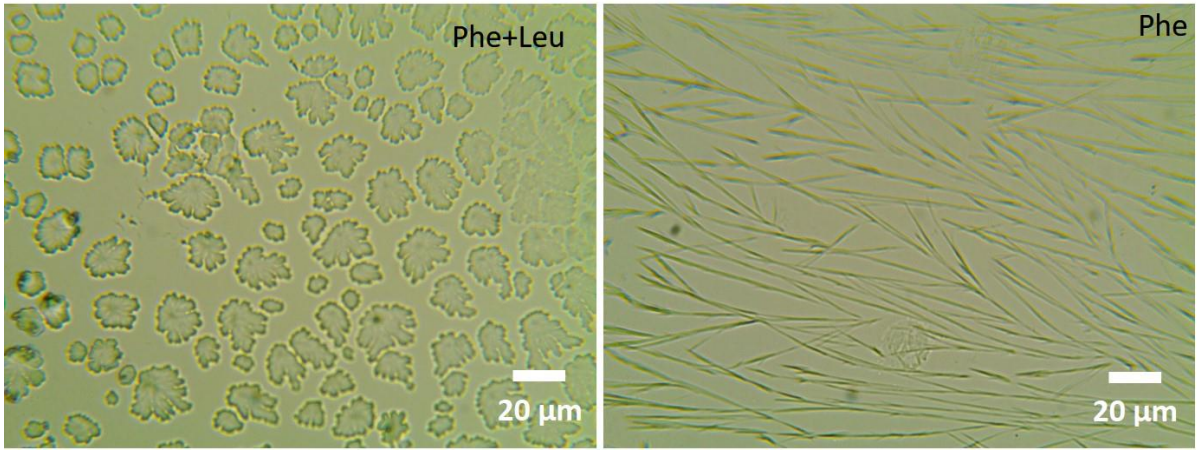

Figure S25: - Optical images for self-assembly of co-assembled phenylalanine:leucine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

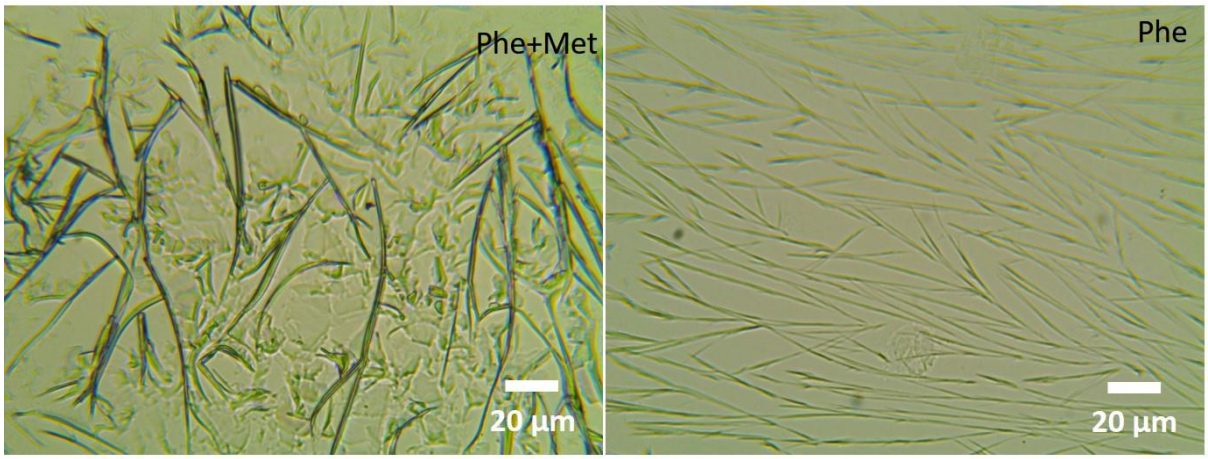

Figure S26: - Optical images for self-assembly of co-assembled phenylalanine:methionine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

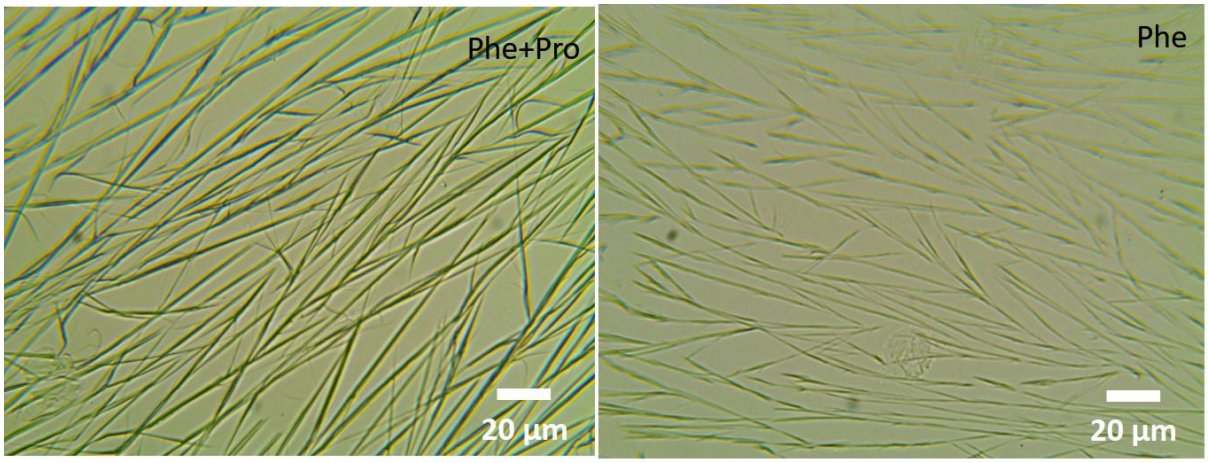

Figure S27: - Optical images for self-assembly of co-assembled phenylalanine:proline (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

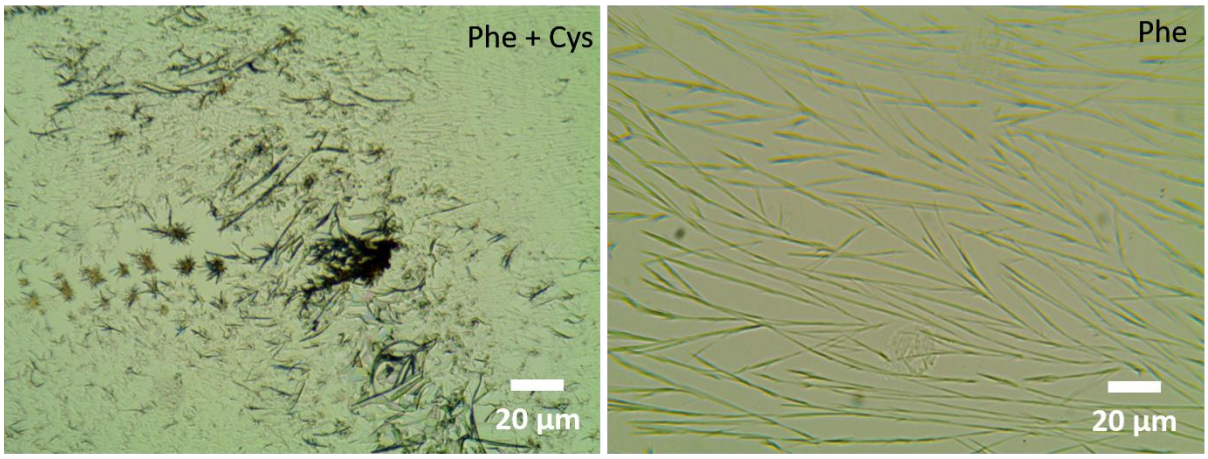

Figure S28: - Optical images for self-assembly of co-assembled phenylalanine:cysteine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

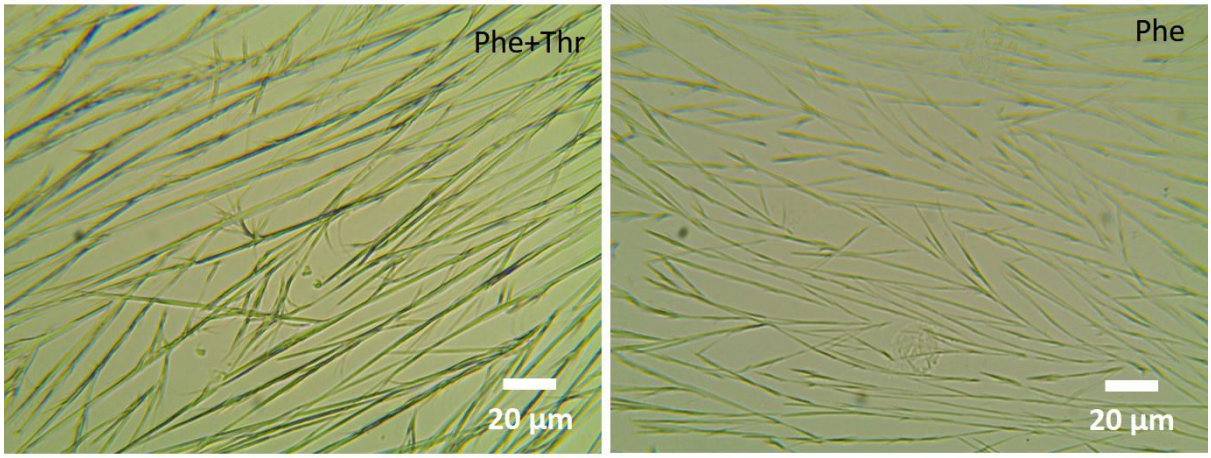

Figure S29: - Optical images for self-assembly of co-assembled phenylalanine:threonine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

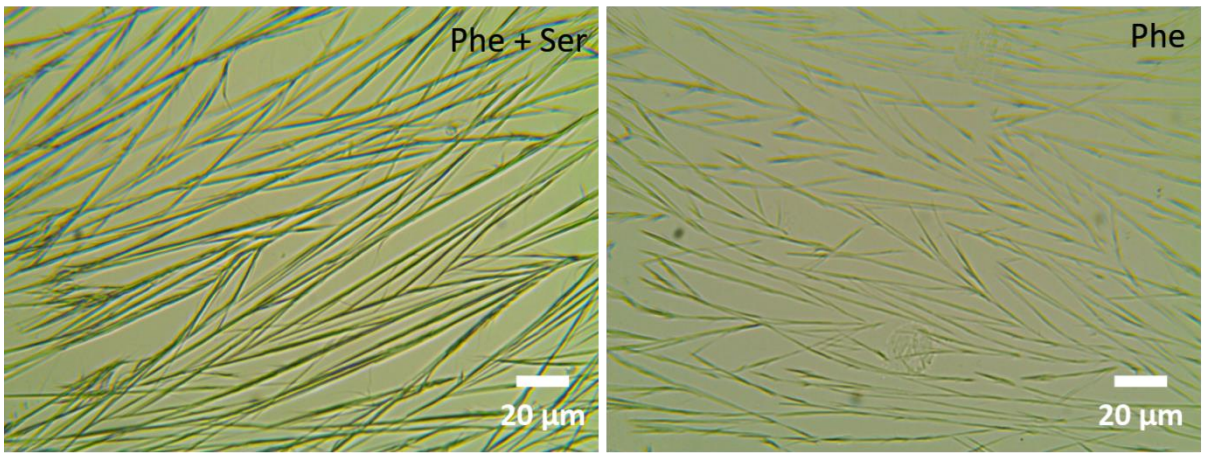

Figure S30: - Optical images for self-assembly of co-assembled phenylalanine:serine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

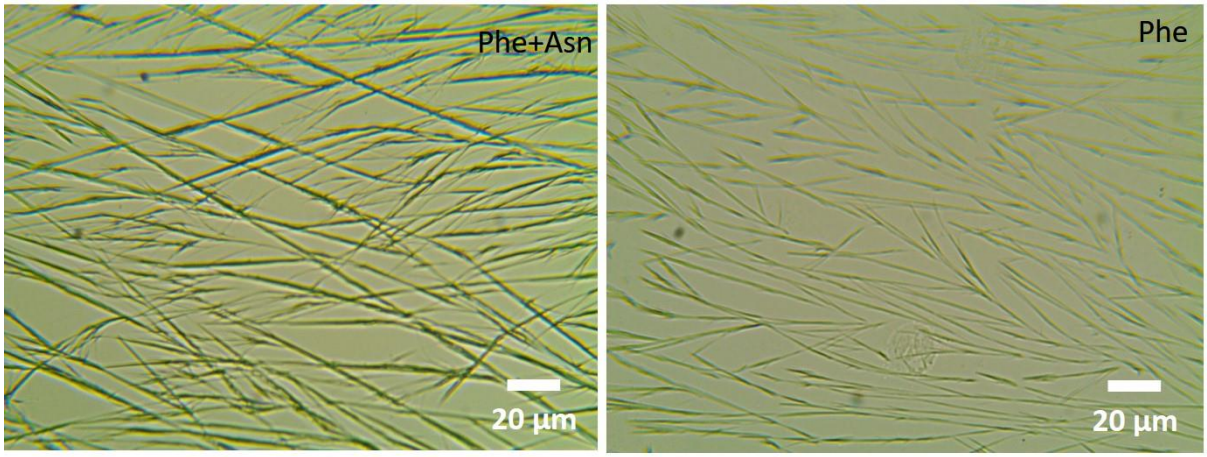

Figure S31: - Optical images for self-assembly of co-assembled phenylalanine:asparagine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

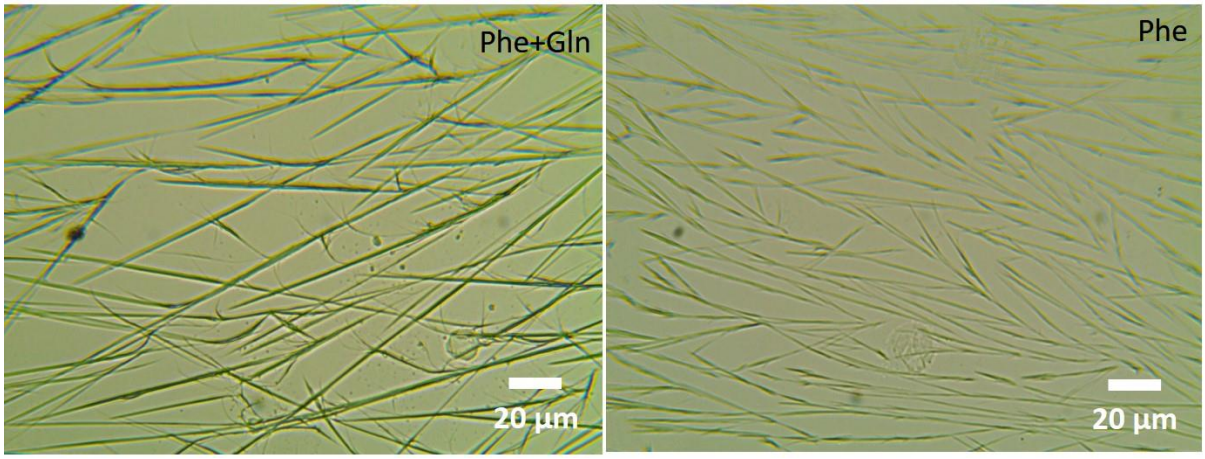

Figure S32: - Optical images for self-assembly of co-assembled phenylalanine:glutamine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

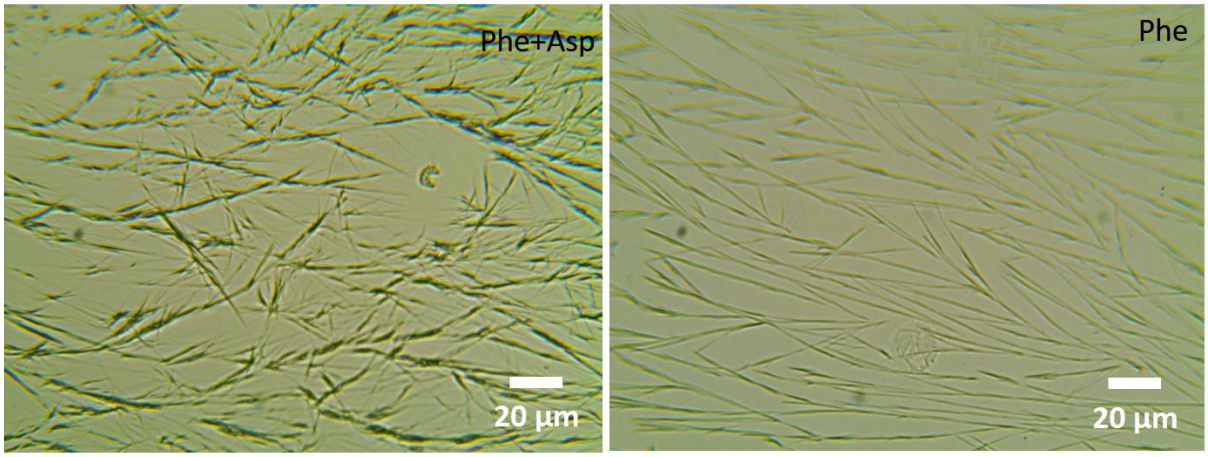

Figure S33: - Optical images for self-assembly of co-assembled phenylalanine:aspartic acid (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

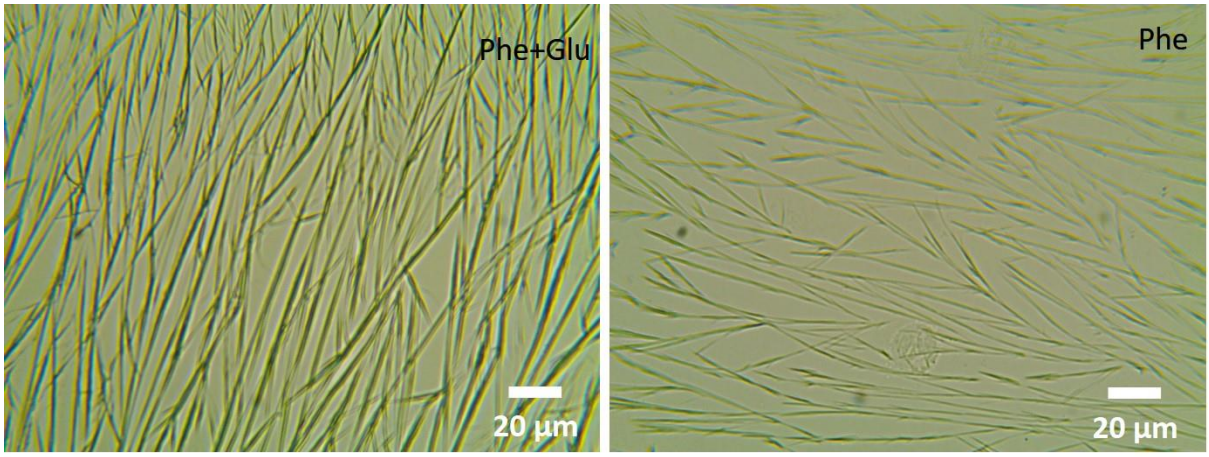

Figure S34: - Optical images for self-assembly of co-assembled phenylalanine:Glutamic acid (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

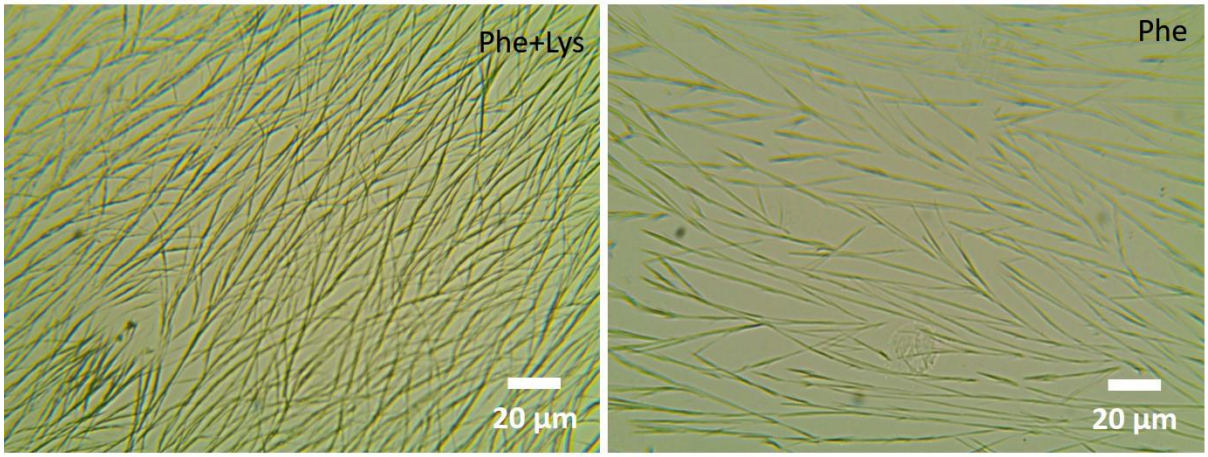

Figure S35: - Optical images for self-assembly of co-assembled phenylalanine:lysine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

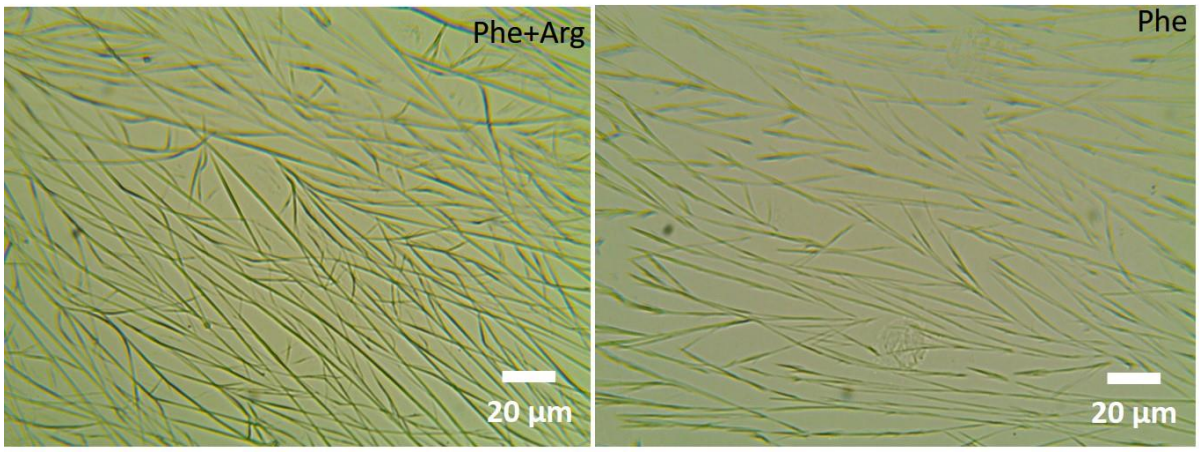

Figure S36: - Optical images for self-assembly of co-assembled phenylalanine:arginine (1mg/mL and 0.5 mg/mL, respectively) and only phenylalanine in aqueous medium

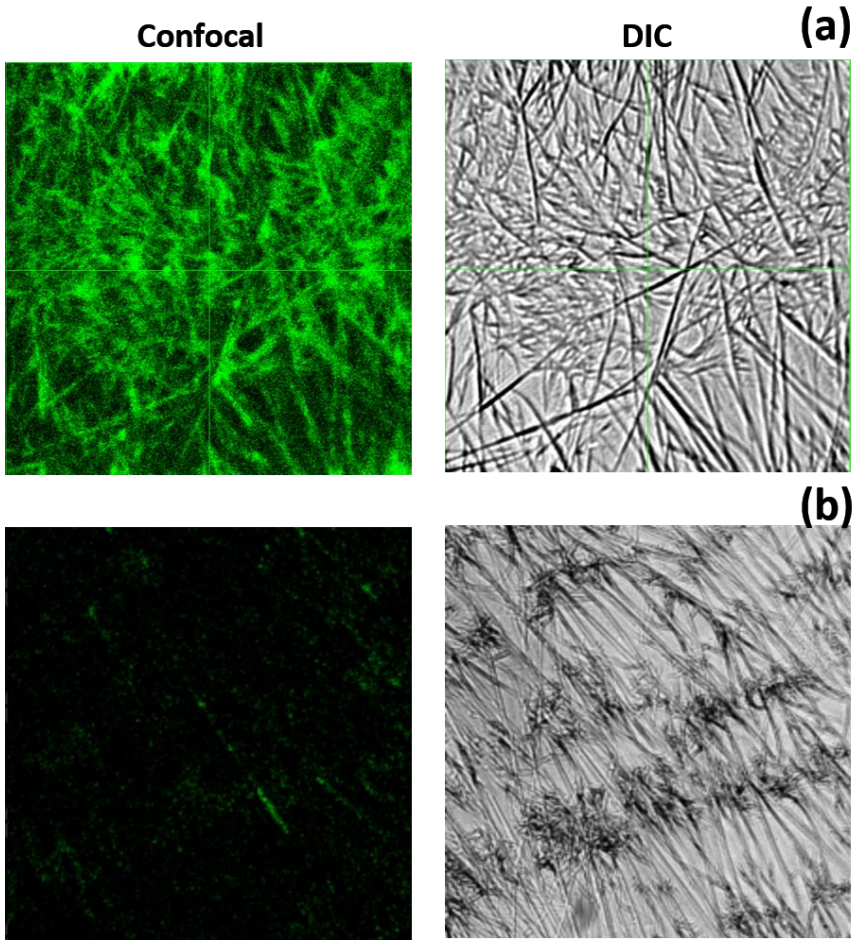

Figure S37: - Deposited phase ThT binding assay for phenylalanine fibrils (a) and Phenylalanine and Leucine (1:0.5 mg/mL) co-assembly state (b).